Synthesis, Spectroscopic Studies and Structure of Gold (III) Chloride Compounds of Heterocyclic N-oxide Diadducts Revealing Short Hydrogen Bond

by

Saud A.Aziz Al-Hamoud

A Thesis Presented to the

FACULTY OF THE COLLEGE OF GRADUATE STUDIES

KING FAHD UNIVERSITY OF PETROLEUM & MINERALS

DHAHRAN, SAUDI ARABIA

In Partial Fulfillment of the
Requirements for the Degree of

MASTER OF SCIENCE

In

CHEMISTRY

May, 1985

Order Number 1355723

Synthesis, spectroscopic studies and structure of gold(III) chloride compounds of heterocyclic N-oxide diadducts revealing short hydrogen bond

Al-Hamoud, Saud A. Aziz, M.S.

King Fahd University of Petroleum and Minerals (Saudi Arabia), 1985

U·M·I
300 N. Zeeb Rd.
Ann Arbor, MI 48106

University of Petroleum and Minerals

Synthesis, Spectroscopic Studies and Structure of Gold(III) Chloride Compounds of Heterocyclic N-oxide Diadducts Revealing Short Hydrogen Bond

BY

Saud A.Aziz Al-Hamoud

A Thesis Presented to the
FACULTY OF THE COLLEGE OF GRADUATE STUDIES

In Partial Fulfillment of the
Requirements for the Degree of

MASTER OF SCIENCE IN

CHEMISTRY

May 1985

UNIVERSITY OF PETROLEUM AND MINERALS

Dhahran, Saudi Arabia

This thesis, written by Mr. Saud A.Aziz Al-Hamoud under the direction of his Thesis Committee, and approved by all its members, has been presented to and accepted by the Dean, College of Graduate Studies, in partial fulfillment of the requirements for the degree of Master of Science in the Chemistry.

Dean
College of the Graduate Studies

Date: 8/6/1985

28.5.85

Department Chairman

Thesis Committee

613169-616221

15/5/85
Dr. Mohammed Sakhawat Hussain
Chairman

25/5/85
Dr. Hassan A.Tayim
Member

15.5.85
Dr. Mazharul Haque
Member

28/5/85
Dr. Mohammed Zamil El-Faer
Member

Dedicated to My

PARENTS AND WIFE

ACKNOWLEDGEMENT

All praise and thanks be to Almighty Allah, first and last, who made every task easy for us.

I wish to express my sincere thanks to my thesis advisor, Dr. M. Sakhawat Hussain for his constant guidance, help and encouragement without which this work could not be completed. All useful suggestions on the draft of the thesis from other members of the thesis committee are acknowledged. I am also thankful to the Chairman Department of Chemistry for his moral support during the course of this investigation.

The Graduate Assistantship by the University of Petroleum and Minerals and support from the Data Processing Center of UPM are gratefully acknowledged.

Table of Contents

LIST OF TABLES

LIST OF FIGURES

الخـــلاصـــة

هذه الدراسة تشمل تصنيع و بيان التركيب الكيميائي للمركبات الناتجة من تفاعل كلوريد الذهب الثلاثي مع أكاسيد البيريدين المستبدلة لينتج مركبات كاتيونية مزدوجة من هذه الاكاسيد تحتوي على رابطة هيدروجينية قوية .

لقد تم تحليل هذه المركبات بالطرق التحليلية و المطيافية المعتادة مثل التحليل العنصري و التحليل باستخدام الاشعة المختلفة من فوق بنفسجية و مرئية و تحت حمراء . و لقد تم ايضا انجاز التحليل البللورى ذو الثلاثة أبعاد لثلاثة مركبات فقط من الستة المحضرة في دراستنا هذه . و تعتبر هذه الرابطة من أقوى الروابط الهيدروجينية المعروفة و الرابطة الهيدروجينية القوية في حالة مركب ثنائي البيكولين المزدوج تعتبر منفردة حيث لا يوجد أى تماثل يربط بين شطرى المركب كما هو الحال في ثلاثي و رباعي البيكولين المزدوج و في معظم المركبات الاخرى المشابهة .

يستدل على وجود الرابطة الهيدروجينية القوية في هذه المركبات ،وجود امتصاص قوى في مجال الاشعة تحت الحمراء عند ١٠٥٠ سم$^{-1}$ ، و المسافة بين ذرتي الاكسيجين تكون أقل من ٢٫٥ أنغ ، و الرنين المغناطيسي البروتوني ما بين ١٠ – ١٨ جزء من المليون ، لقد بذلت جهود لبيان العلاقة بين المجموعات المستبدلة على حلقة البنزين و الاثر الحثي لهذه المجموعات .

و أخيرا فان أكاسيد البيريدين المستبدل تصلح كمواد مفيدة جدا في استخلاص الذهب نظرا لكبر معامل الانتشار لهذه الاكاسيد .

ABSTRACT

The present study deals with the synthesis and structure elucidation of several noval gold(III) chloride compounds having general formula $[H(R\text{-}pyNO)_2][AuCl_4]$ where R = 2-Me, 3-Me, 4-Me 2,6-$(CH_3)_2$, p-NO_2 and m-COOH. All compounds were characterized by the usual analytical and spectroscopic techniques, such as elemental analysis, ultraviolet, visible, infrared and proton-N.M.R. spectra. The three-dimensional single crystal x-ray structure analysis was completed on three compounds, namely, $[H(2\text{-}picNO)_2][AuCl_4]$, $[H(3\text{-}picNO)_2][AuCl_4]$ and $[H(4\text{-}picNO)_2][AuCl_4]$.

In all compounds the short hydrogen bonded dimeric cation was stabilized by the $[AuCl_4]^-$ anion. The O-H-O bond in the diadducts is among the shortest so far reported in literature. The short hydrogen bond in the $[H(2\text{-}picNO)_2][AuCl_4]$ is unique in that the bridged proton has no symmetry restrictions usually known to exist in similar hydronium ion diadducts. The energetics of the O-H-O linkage were explained in terms of the chemical potentials and the O...O separation.

The presence of a strong and broad absorption band around 1050 cm^{-1} in IR spectra has been establishes as a diagnostic observation for the existence of a short hydrogen bond with O...O separation less than 2.5Å. Similarly, a δ-shift of 10.0 to 18.0 p.p.m. is usually observed for the resonance of the bridged proton in these intramolecular short hydrogen bonded species.

Efforts were made to explain the spectroscopic and crystallographic results in terms of inductive effects of the substituents on the aromatic N-oxides.

Substituted pyridine N-oxides are potentially useful reagents for extraction and photometric determination of gold because of the quantitative separation and the high extinction coefficients of the products formed. The present study will aid in developing an extractive-photometric procedure for estimation of gold. The present work is a part of the ongoing research programme dealing with the chemistry of compounds having short (or strong) hydrogen bond.

CHAPTER ONE

1. LITERATURE REVIEW

The oxygen atom of the N-oxide group is more polar than it is in other common oxo donors such as alcohols, ethers and amides as indicated by dipole moment [1-3] and thermodynamics studies [4] of compounds having N-oxide group. In aromatic amine oxides the oxygen $2p\pi$ electrons are conjugated with the aromatic ring [1-3,5-6] and the basicity of these N-oxides can be systematically varied by appropriate substitution on the aromatic ring with concomitant minimal changes in steric interaction at the reaction site. These properties of the heterocyclic amine N-oxides have greatly contributed to the coordination chemistry utilizing these ligands [7-8].

1.1: Coordination Chemistry of Heterocyclic N-oxides (A Brief Survey)

Heterocyclic N-oxides mainly form two types of compounds :

Type (A): Compounds with the N-oxides acting as monodentate, bridging or chelating ligands coordinating to the metal through the N-O oxygen atom.

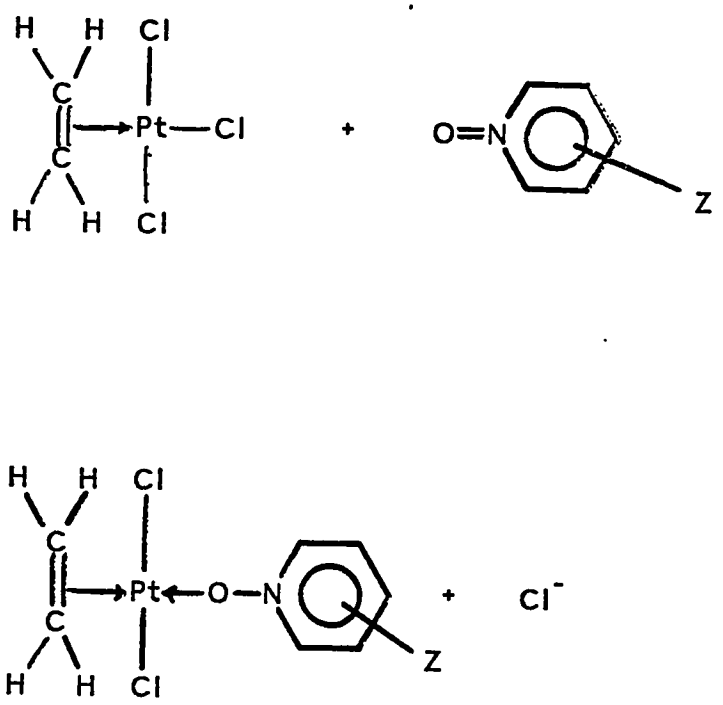
Type (B): Diadducts of the N-oxide, analogous to $[H_5O_2]^+$ ion, which are formed as a short hydrogen-bonded hydrogen(1^+) ion, normally stabilized by a large anion.

The compounds of Type (A) are quite common [7-8] whereas those of Type (B) are not widely known. Some typical examples of each type are given in the following.

Type (A): Compounds with Heterocyclic Amine N-oxides as Monodentate, Bridging or Chelating Ligands.

Monofunctional donor coordination through oxygen of the aromatic amine oxides usually gives octahedral compounds with a wide variety of transition metals [7-8], although it has been stated [9] that only a single example was known before 1961. These hexakis (aromatic N-oxide) compounds of the types $M(pyNO)_6X_2$ or $M(pyNO)_4X_2$ (pyNO = pyridine N-oxides and M = Cu(II), Zn(II), Ni(II)) are quite common and the diversity of compounds and compound types is illustrated in reported literature [8]. Several of these compounds exhibit Jahn-Teller effect and are the subject of recent spectroscopic and E.S.R studies [10-11]. The maximal metal coordination is normally achieved with metal perchlorates whereas anions of greater coordinating ability than perchlorates are not easily replaced by heterocyclic N-oxides and products of different stoichiometries were obtained.

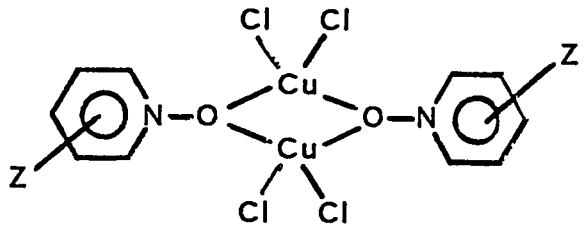
Another series of compounds [12] with monodentate N-oxide are the mono-pyNO compounds formed when $K[Cl_3PtC_2H_4]$, Zeise's salt, was stirred with the N-oxides to form the compound (I) as shown in the equation below [12-13], (pyNO does not react with K_2PtCl_4 in aqueous solution even when stirred for several days).



(I)

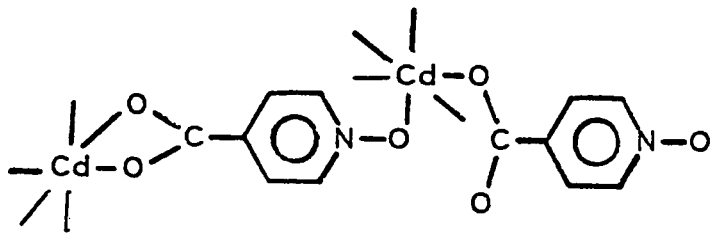
The above type of platinum, palladium and rhodium complexes have been isolated and characterized[12].

The aromatic amine N-oxides can also act as a bridging group and bi- or polynuclear compounds having structure (II) are known [14] with pyNO and many of its derivatives.



(II)

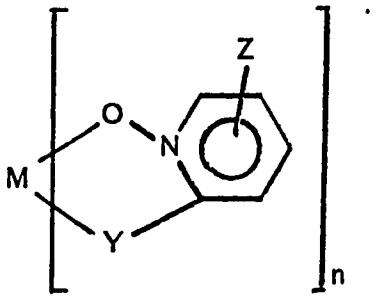
Another interesting structure of the bridging type is of recently studied $[Cd(pCOOH\text{-}pyNO)_2(H_2O)]_n$ compound (III), in which coordination occurs through the N-O oxygen and one of the (COO) oxygens,



(III)

with ligand, thus, forming a double bridge between Cd^{2+} ions. The structure is an endless chain stretching diagonally through the unit cell [15].

Suitable α-substituted aromatic N-oxides act as bidentate ligands and lead to the formation of chelate compounds containing the structural entity (IV), where M = an acidic site, generally a metal ion, and y = groups such as $-NH_2$, -OH,-SH, $-CO_2H$.



(IV)

Thus, 2-hydroxy, 2-mercapto, 2-carboxypyridine N-oxides readily form compounds with transition metal ions in which the donors act as bidentate ligands [16-17]. However, with 2-aminepyridineN-oxide [18] the usual compound of the type $ML_6(ClO_4)_2$ is formed with the ligand acting in a monodentate fashion when the 2-amine pyNO is mixed with methanolic solution of the metal perchlorates.

Type (B): Short Hydrogen Bonded Dimeric Cationic Compounds.

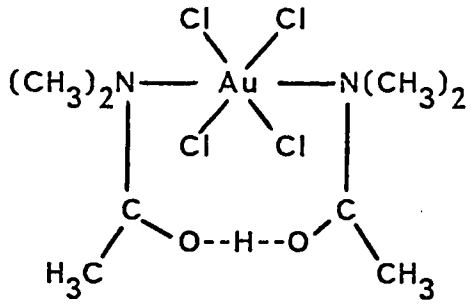
The dimeric cations having hydrogen bonded heterocyclic N-oxides have not been extensively studied. Although, several cations, analogous to the well-known $[H_5O_2]^+$ [19], of the type $[BHB]^+$ where B = $(CH_3)_2NCO(CH_3)$, Et_2O or Ph_3PO are known [20-23], only a few such cations for aromatic amine N-oxides are reported [24-27]. These cations are formed when the N-oxides combines with a strong acids in the base : acid ratio of 2 : 1.

The corresponding pyridinium-pyridine ions $[H(C_6H_5N)_2]^+$ were reported [28-29] in various salts and attempts were made [30-31] to interpret spectroscopic data of these ions in terms of various models for the potential functions associated with short hydrogen bonds. Two basic salts of 2-picNO (picoline N-oxide), namely $[H(2\text{-picNO})_2]Br$ and

$[H(2\text{-picNO})_2]Cl.2H_2O$ are also known [25,26] but a definite structure analysis of the first could not be completed because of the crystal being damaged by exposure to x-rays, whereas the structure of the second, called Dunlop's salt, was explained on the basis of a disorder across the twofold axis of the crystal.

1.2: Objectives of the Present Work.

The present research grew out of the work of Ziegler et. al. [32] reporting the synthesis of a six-coordinate gold(III) compound, $H[(dma)_2AuCl_4]$ (dma = dimethylacetamide), for which structure (V) was proposed.



(V)

Ziegler also reported [33] extractive-photometric determination of gold(III) with pyridine N-oxide, again assuming the formation of a six-coordinate gold(III) compound, $H[AuBr_4(pyNO)_2]$, for the resulting species in solution. Since six-coordinate gold(III) compounds are not common, Hussain and Schlemper [21] investigated the structure of $H[AuCl_4(dma)_2]$ by neutron and x-ray diffraction, in order to confirm structure (V) which was originally proposed on the basis of spectroscopic data (i.r. and ^1H n.m.r)

alone. The single crystal structural analysis revealed that dma molecules in $H[(dma)_2AuCl_4]$ form a dimeric cation $[H(dma)_2]^+$ and were no where close to the gold atom. Thus, the assumption of six-coordinate gold(III) through coordination of nitrogen of dma was proved to be erroneous because the i.r. and ^1H n.m.r spectra would not differentiate between structure (V) and the ionic species $[H(dma)_2]^+[AuCl_4]^-$, having 6- or 4-coordinate gold(III), respectively. The structure analysis by Hussain and Schlemper [24] of gold(III)-Pyridine N-oxide also revealed 4-coordinate gold(III) with actual structure being $[H(pyNO)_2][AuCl_4]$, in contrast to $H[AuBr_4(pyNO)_2]$ proposed by Ziegler [33] for the corresponding bromo compound, but in agreement with a similar compound of the formula $[H(thf)_2][AuCl_4]$, later proposed by Ziegler [34] for the tetrahydrofuran (thf) adduct. In the above two compounds, namely $[H(dma)_2][AuCl_4]$ and $[H(pyNO)_2][AuCl_4]$, the hydrogen bonded dimeric cation exhibits O---O distances of 2.43(2) and 2.41(1)Å which are 'very short' for a hydrogen bond.

The O---O distance should be about 3.3Å on the simple basis of the sum of the van der Waals radii of the atoms involved in an approximately linear O-H-O bonding. The O---O distance in ice is 2.7Å and hydrogen bonds having O---O distance greater than 2.7Å are called to be "long", those less than 2.7Å and greater than 2.5Å are "short" and those less than 2.5Å are "very short" [20]. The increasing strength of hydrogen bonds as O---O diminishes is reflected in their dissociation energies. While the energy of a "long bond" may be less than 2 kcal/mole, energies far exceeding 10 kcal/mole, attach to "very short" bonds.

In view of the above findings, a systematic study was undertaken to investigate the interaction of heterocyclic N-oxides with gold(III) keeping the following specific objectives in view.

1- Search for Open Symmetry-free Short Hydrogen Bond.

The majority of the $[H_5O_2]^+$-type cations are centrosymmetric i.e the hydrogen atoms in the cations is located at a point of crystal symmetry. It is pointed out [19-20,35-36] that the symmetry-free open short hydrogen bonds with unambiguously defined space groups are rare in the case of the dimeric cations. This is in contrast to several chelate structures studied by Hussain and Schlemper [37-42], where intramolecular short hydrogen bonds are always symmetry-free. However, shortness of O---O separation in the chelate structures can be interpreted to be due to the compression in the intramolecular short hydrogen bond. One of our objectives was to screen systems for additional examples of open and symmetry-free short hydrogen bonds to understand the chemical potential in which the hydrogen sits because in the symmetry-restricted bond the crystallographic restrictions on the bridged hydrogen often obscure such understanding and doubts have been raised [43-44] as to the centricity of the hydrogen in these cases.

2- Basicity vs Bonding Properties of Aromatic N-Oxides.

As pointed out by Orchin and Schmidt [12], no systematic studies have been carried out to correlate bonding interactions at the reaction site of the aromatic N-oxides with the changes in basicity by appropriate substitution on the aromatic ring. We have attempted to fill this gap and efforts

are made to explain the infrared and crystallographic results in terms of inductive effects of the substituents on the aromatic N-oxides. We were also interested in investigating whether or not the aromatic N-oxides of altogether different basicity and steric requirement than that of pyNO will effect halogen substitution in $[AuCl_4]^-$ ion to form stable gold(III) compounds.

3- Reagents for Extractive-Photometric Determination of Gold.

The compounds of gold(III) with aromatic N-oxides are significant in their own right because of the importance of similar compounds in selective extractive-photometric determination of gold [33]. The solution chemistry and solid state structures of these compounds may also serve as chemical models for understanding the chemistry of gold drugs used in Chrysotherapy (gold treatment) [45-49].

4- Free-Rotation in the Diadducts.

Both symmetry free and symmetry-restricted hydronium ion diadducts of heterocyclic N-oxides possess free rotation along the O---O axis and are interesting molecular systems for theoretical studies predicting most stable orientation of the heterocyclic rings in solution or in the solid state. The influence of packing forces on various rotational conformations in the solid state can be studied from the crystallographic results.

CHAPTER TWO

2. EXPERIMENTAL SECTION

2.1: Chemicals and Solvents.

All chemicals and deuterated solvents were of analytical or spectral grade quality, obtained from Fluka Chemical Company and were used without any further purification.

2.2: Synthetic Procedures.

2.2.1: General Method of Preparation.

The ligand was dissolved in a minimum amount of methanol and an aqueous slurry of chloroauric acid was added, keeping a gold(III):ligand ratio of 1:2. In most cases yellow crystalline product immediately formed, which was filtered off and redissolved in an excess of methanol to obtain a clear yellow solution. This solution was allowed to evaporate under nitrogen in a dry box to give well-formed yellow crystals which were separated from solution by decantation. If no residue was formed upon the initial mixing of the $HAuCl_4$ and the ligand solutions, the resulting solution was filtered and allowed to evaporate slowly under nitrogen untill crystals of the product appeared. These crystals were harvested in several batches from the solution. Prolonged exposure of the solution to open atmosphere resulted in the formation of fine particles of metallic gold, which could be prevented by addition of a few drops of dilute HCl and avoiding prolonged exposure of the solution to atmosphere. The compounds which precipitated immediately on mixing could also be prepared by using an HCl solution of $NaAuCl_4$ instead of $HAuCl_4$, and washing the residue with a very small volume of

methanol-water solution to remove any sodium chloride. The yield from the latter procedure was very low. Elemental analyses of the products were performed on a Carlo Erba (Italy) Elemental Analyzer Model 1106. Individual methods of preparation are given below and the results of the elemental analysis are shown in Table I.

2.2.2: Individual Methods of Preparation and Crystal Growth.

(1) Bis(2-picoline N-Oxide)hydronium Tetrachloroaurate(III):

$[H(2\text{-picNO})_2][AuCl_4]$

The compound was prepared by mixing a methanolic solution of 0.54 g (4.95 mmol) of 2-Picoline N-oxide and 0.400 g of aqueous solution of $HAuCl_4$. A yellow colored precipitate was immediately formed which was slowly dissolved in methanol until the total volume of the solution was about 30 ml. Another 0.050 g of 2-Picoline N-oxide was added to keep the ligand in excess. The yellow crystals of the compound were obtained by evaporation of the above solution under nitrogen over a period of 2-3 days.

(2) Bis(3-picoline N-Oxide)hydronium Tetrachloroaurate(III):

$[H(3\text{-picNO})_2][AuCl_4]$

The compound was prepared by mixing a methanolic solution of 0.70 g of 3-Picoline N-oxide and 0.43 g of $HAuCl_4$ dissolved in a minimum amount of water. The resulting solution was acidified with 4-5 drops of dilute HCl. A yellow colored solid was immediately formed which was recrystallized from methanol.

(3) Bis(4-picoline N-Oxide)hydronium Tetrachloroaurate(III):

$[H(4\text{-picNO})_2][AuCl_4]$

The $[H(4\text{-picNO})_2][AuCL_4]$ was prepared by mixing 0.540 g (4.95 mmol) of 4-picNO and 0.400 g of $HAUCL_4$, both dissolved in a minimum amount of methanol. Yellow colored precipitate was obtained from which crystals were obtained by slow evaporation of its methanol solution having a slight excess of 4-picNO under nitrogen.

(4) Bis(p-nitro pyridine N-Oxide)hydronium Tetrachloroaurate(III):

$[H(pNO_2\text{-}pyNO)_2][AuCl_4]$

0.55 g of p-nitro pyridine N-oxide was slowly dissolved in methanol with continuous stirring untill all the sample dissolved. The resulting solution was filtered and mixed with 0.15 g of $HAuCl_4$ which was dissolved in a minimum amount of methanol to obtain about 35 ml of the total solution. Crystals were grown from this solution by evaporation over a period of a week in a 100 ml conical flask.

(5) Bis(nicotinic acid N-oxide)hydronium Tetrachloroaurate(III):

$[H(mCOOH\text{-}pyNO)_2][AuCl_4]$

100 mg (0.266 mmol) of $HAuCl_4$ dissolved in a minimum amount of water and acidified with 6 drops of concentrated HCl, was mixed with 43.0 mg (0.6 mmol) of nicotinic acid (N-oxopyridine-3-carboxylic acid) which was dissolved in a minimum amount of methanol . No residue was formed upon mixing. The resulting solution was filtered in a flask and left for several days for crystallization.

(6) Bis(2,6-dimethylpyridine N-Oxide)hydronium Tetrachloroaurate(III): $[H(2,6\text{-}(CH_3)_2pyNO)_2][AuCl_4]$

The $[H(2,6\text{-}(CH_3)_2pyNO)_2][AuCl_4]$ was prepared by mixing 0.07 g of the (2,6-dimethyl pyridine N-oxide) and 0.100 g of $HAuCl_4$, both dissolved in a minimum amount of methanol. Yellow colored precipitate was formed from which crystals were obtained by the slow evaporation of methanol solution having a slight excess of the ligand.

Table I: Results of Elemental Analyses for Gold(III) Chloride Compounds of Heterocyclic N-oxides.[a]

Compound	M.Pt. (°C)	%C	%N	%H
$[H(2\text{-picNO})_2][AuCl_4]$	141	25.4(25.8)	5.0(5.0)	2.8(2.7)
$[H(3\text{-picNO})_2][AuCl_4]$	95	26.3(25.8)	5.2(5.0)	2.9(2.7)
$[H(4\text{-picNO})_2][AuCl_4]$	103	25.0(25.8)	5.0(5.0)	2.7(2.7)
$[H(pNO_2\text{-pyNO})_2][AuCl_4]$	169	20.1(19.4)	9.5(9.0)	1.5(1.5)
$[H(mCOOH\text{-pyNO})_2][AuCl_4]$	184	20.9(23.3)	3.3(4.5)	1.6(1.8)
$[H(2,6\text{-}(CH_3)_2pyNO)_2][AuCl_4]$	181	29.1(28.7)	4.8(4.8)	3.2(3.2)

(a) The calculated values are given in parentheses.

2.3: Spectroscopic Measurements.

2.3.1: Ultraviolet and Visible Spectra.

The electronic absorption spectra in the region 190-750 nm for all compounds were obtained on a Beckman Acta MVII spectrophotometer using a 1-cm cell and a dilute solution of the compound in spectral grade methanol. The ultraviolet spectra were sometimes used to identify product formation in solution. The electronic spectral data are listed in Table II and some representative spectra are shown in Figures 1 to 3.

2.3.2: Infrared Absorption Spectra.

Infrared spectra of KBr discs of perfectly dried samples were obtained on a Perkin Elmer 180 spectrophotometer. Efforts were made to obtain pellets of uniform thickness for the infrared spectral measurements using the usual hydraulic press. All relevant infrared absorption peaks are listed in Table III and some representative spectra are shown in Figures 4 to 6.

2.3.3: NMR Measurements.

Proton n.m.r spectra of freshly prepared solutions in solvents such as acetonitrile, nitromethane, methanol and $[^2H_6]$-dimethylsulfoxide(dmso) were obtained on a Varian T60 or on XL-200 n.m.r spectrometer. The chemical shifts of all relevant n.m.r peaks are listed in Table IV, and two representative n.m.r. spectra are shown in Figures 7 and 8.

Table II

Electronic Absorption Spectral Data for Free Heterocyclic N-Oxides and their Gold(III) Chloride Compounds[a].

Compound	Conc. x 10^4 ($M\ L^{-1}$)	λ (nm)	ν (cm^{-1})	ε x 10^4 ($M^{-1}cm^{-1}$)
[2-picNO]	1.67	210	47,619	4.46
		259	38,610	3.30
$[H(2\text{-picNO})_2][AuCl_4]$	0.16	213	46,948	17.7
		(229)[b]	43,668	10.3
		257	38,910	7.93
		321	31,152	1.48
[3-picNO]	1.72	214	46,728	4.18
		263	38,022	3.31
$[H(3\text{-picNO})_2][AuCl_4]$	0.54	220	45,455	16.7
		(227)	44,053	13.4
		262	38,168	10.6
		320	31,250	1.90
[4-picNO]	1.47	207	48,,09	3.89
		264	37,879	3.77
$[H(4\text{-picNO})_2][AuCl_4]$	0.72	216	46,296	10.7
		(227)	44,053	4.56
		264	37,879	5.78
		320	31,250	0.96

Continued on the next page

Table II --(Continued)

Compound	Conc. x 10^4 ($M\ L^{-1}$)	λ (nm)	ν (cm^{-1})	ε x 10^4 ($M^{-1}cm^{-1}$)
[pNO_2-pyNO]	1.26	220	45,455	1.77
		231	43,290	2.17
[H(pNO_2-pyNO)$_2$][$AuCl_4$]	0.28	220	45,455	12.5
		227	44,053	13.9
		325	30,769	11.3
[mCOOH-pyNO]	0.76	221	45,249	6.38
		267	37,453	3.78
		322	31,056	0.31
[H(mCOOH-pyNO)$_2$][$AuCl_4$]	0.09	216	46,296	23.8
		(224)	44,642	17.4
		263	38.023	4.51
		319	31,348	1.93
[2,6(CH_3)$_2$-pyNO]	1.13	216	46,296	0.98
		220	45,455	1.48
		257	38,911	3.05
[H(2,6(CH_3)$_2$-pyNO)$_2$][$AuCl_4$]	0.23	220	45,455	9.62
		(229)	43,668	6.47
		256	39,063	9.97
		320	31,250	0.96

(a) Spectral grade CH_3OH was used as a solvent for in all cases.

(b) The position of shoulders are given in parentheses.

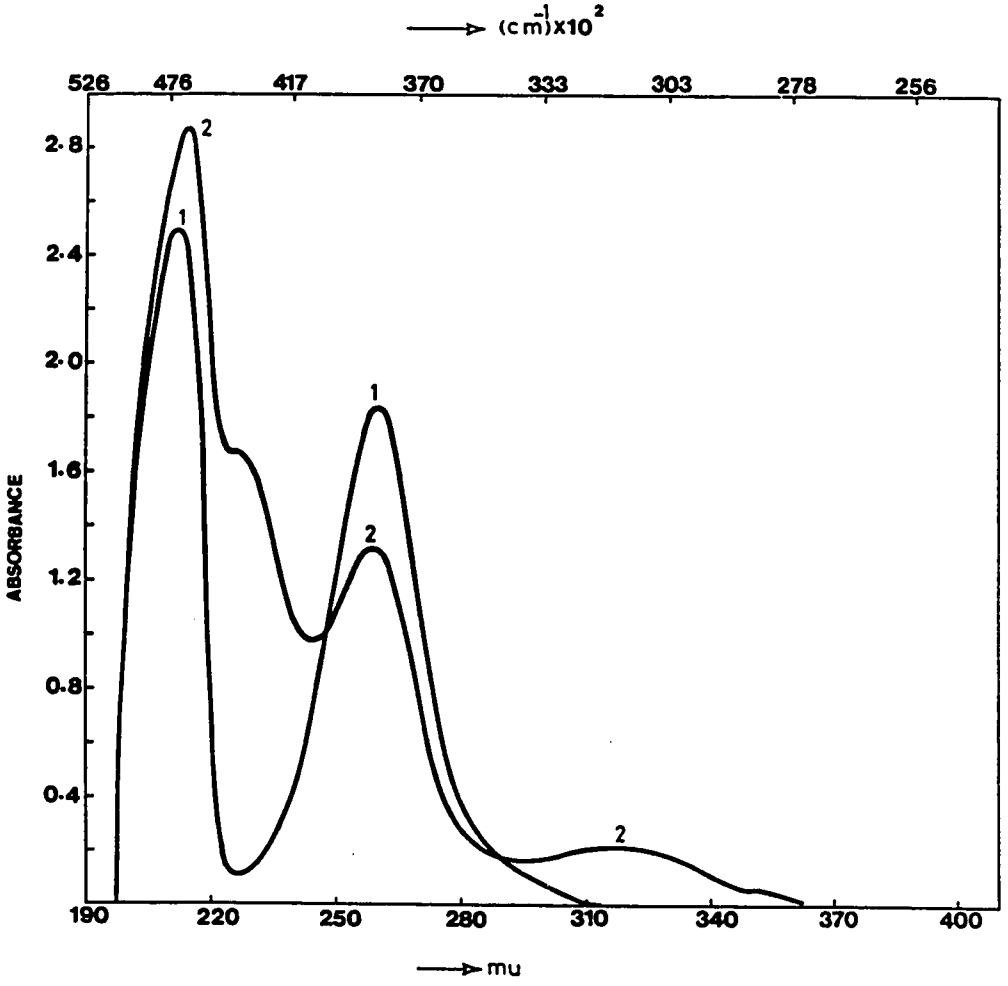


Figure 1: The electronic absorption spectra of: (1) free 2-picoline N-oxide and (2) $[H(2\text{-picNO})_2][AuCl_4]$ in CH_3OH.

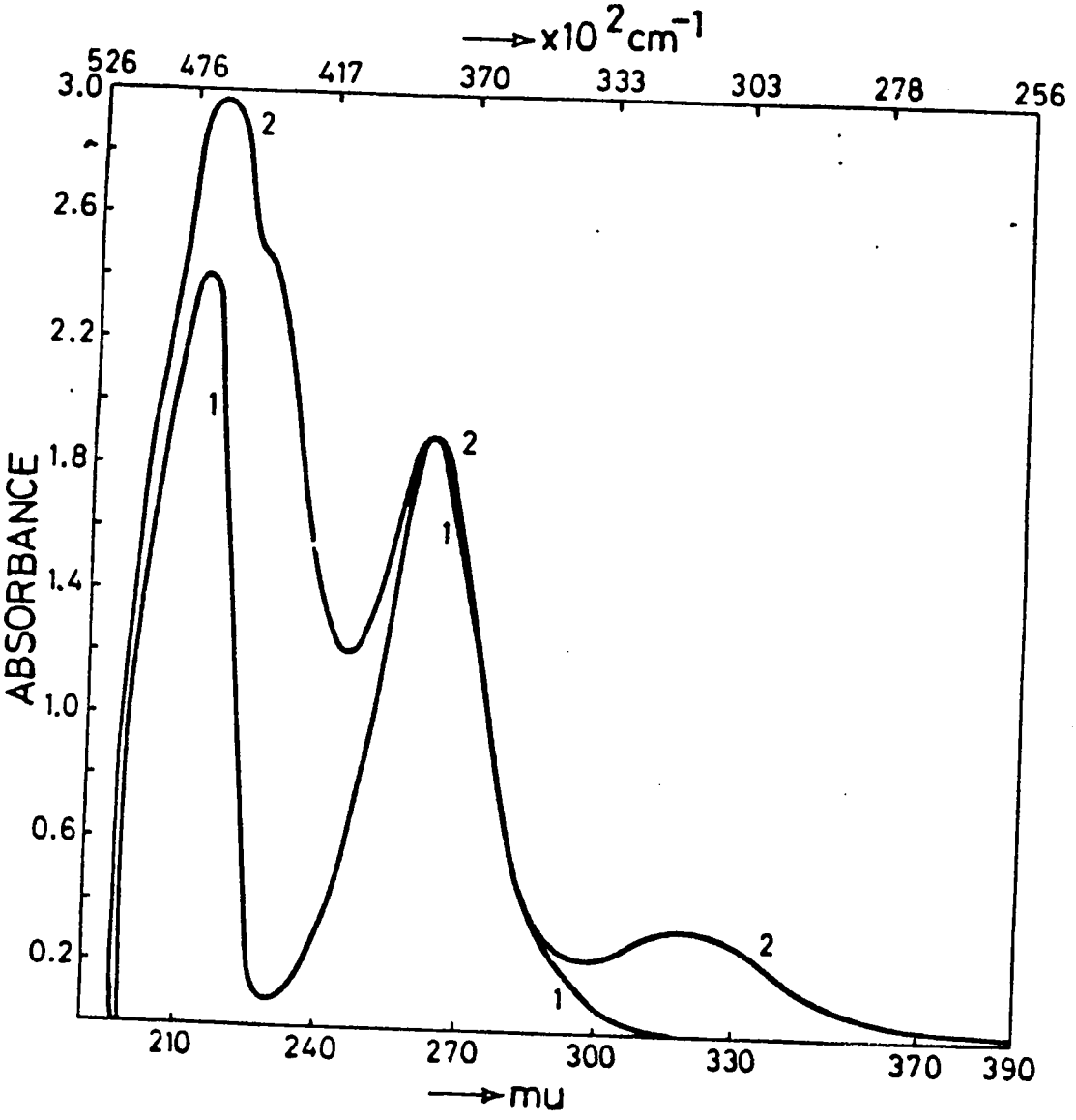


Figure 2: The electronic absorption spectra of: (1) free 3-picoline N-oxide and (2) $[H(3\text{-picNO})_2][AuCl_4]$ in CH_3OH.

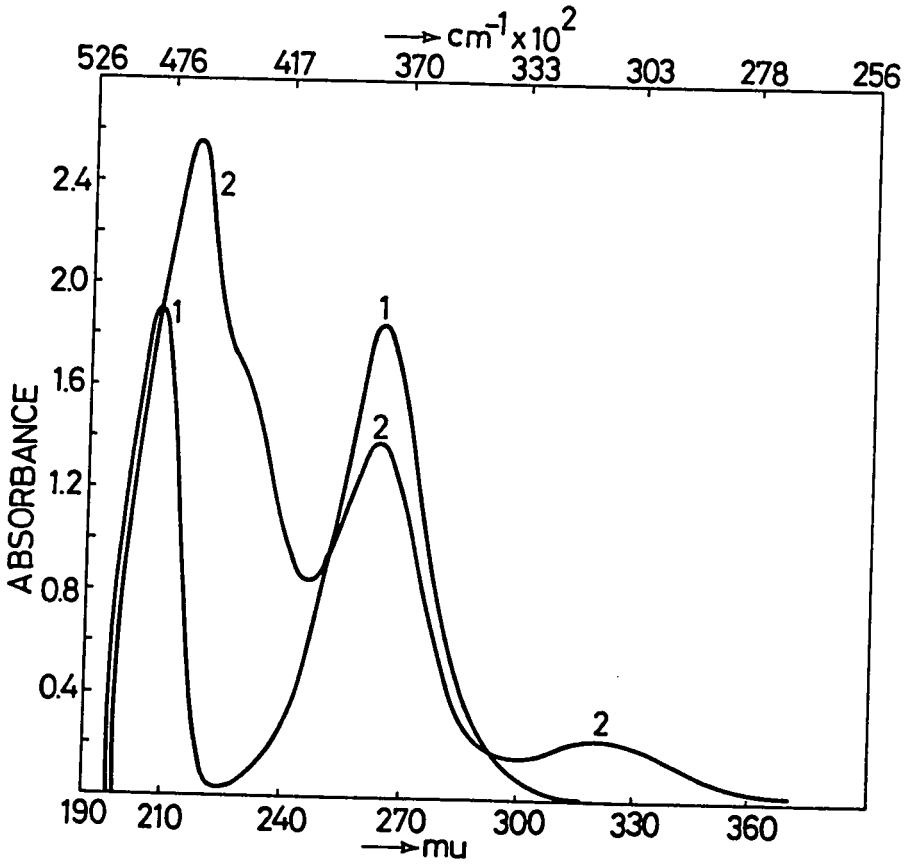


Figure 3: The electronic absorption spectra of: (1) free 4-picoline N-oxide and (2) $[H(4\text{-picNO})_2][AuCl_4]$ in CH_3OH.

Table III

Relevant Infrared Absorptions (cm^{-1}) for the Heterocyclic N-oxides and their Gold(III) Chloride Compounds.

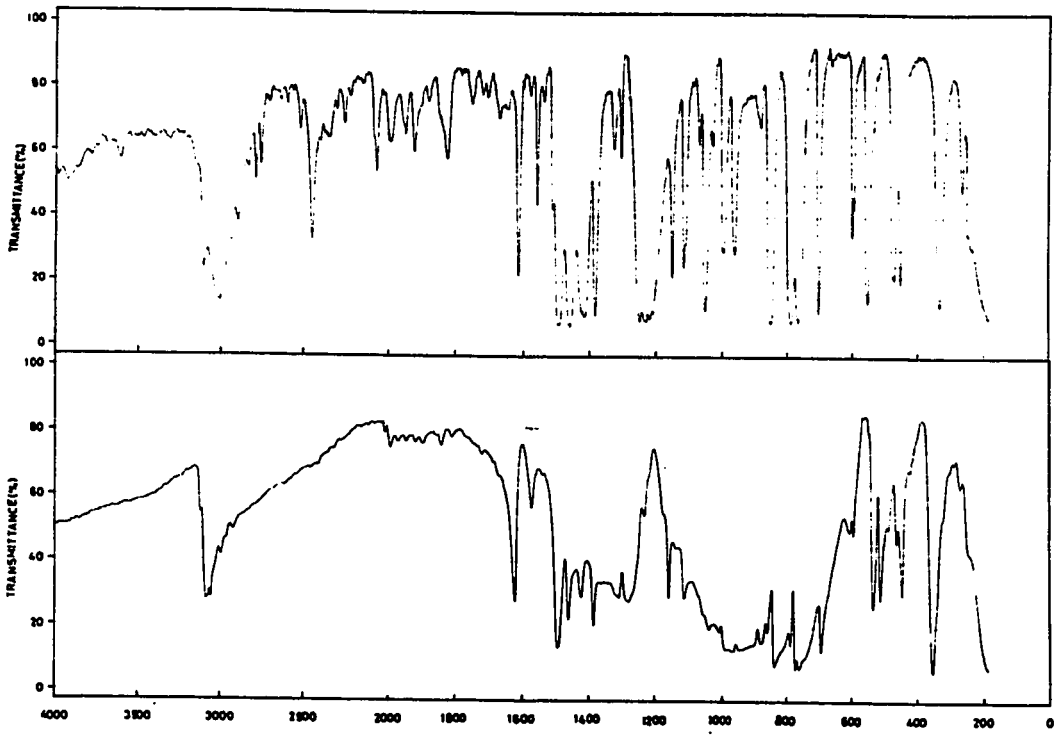
Compound	Above 2800	ν_{N-O}	ν_{O-H-O} [(a)]	Below 560 cm^{-1}
[2-picNO]	3420 3120 3020	1250	-	555 475 450 335 265
$[H(2\text{-picNO})_2][AuCl_4]$	3060	1190	700- 1050	535 510 450 350
[3-picNO]	3380 3050	1270	-	560 520 490 440 305
$[H(3\text{-picNO})_2][AuCl_4]$	3040 3110	1200	750- 1150	545 520 460 425 340 290
[4-picNO]	3410 3090 3010	1250	-	520 480 335
$[H(4\text{-picNO})_2][AuCl_4]$	3080	1200	700- 1050	500 440 340 315

Continued on the next page

Table III --(Continued)

Compound	Above 2800	ν_{N-O}	ν_{O-H-O}	Below 560 cm^{-1}
[pNO_2-pyNO]	3010 3100	1270	-	540 515 460
[H(pNO_2-pyNO)$_2$][$AuCl_4$]	3010 3120	1230	750- 1150	550 480 440 350
[mCOOH-pyNO]	3080	1320	-	570 525 460 420 300
[H(mCOOH-pyNO)$_2$][$AuCl_4$]	3070	1310	830- 1050	565 520 430 355
[2,6(CH_3)$_2$-pyNO]	3400 2920 3050	1240	-	570 510
[H(2,6(CH_3)$_2$-pyNO)$_2$][$AuCl_4$]	2920	1240	700- 1000	560 470 340 280

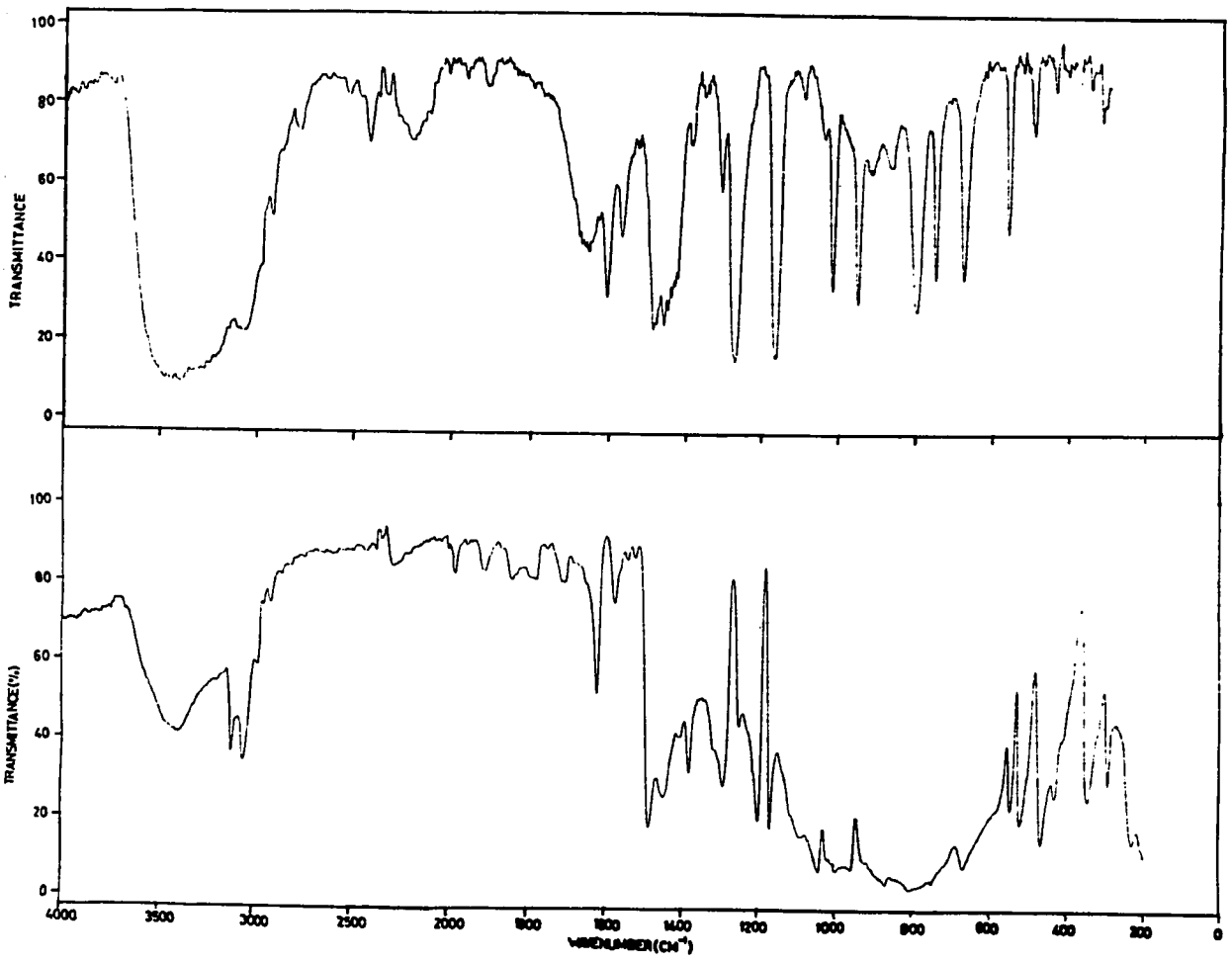
(a) The broad and intense absorption in the region 700-1150 cm^{-1} was overlaid with a number of maxima from free heterocyclic N-oxide.



(1)

(2)

Figure 4: Infrared spectra of: (1) free 2-picNO and (2) $[H(2\text{-picNO})_2][AuCl_4]$ showing the broad absorption for the short O-H-O hydrogen bond.



(1)

(2)

Figure 5: Infrared spectra of: (1) free 3-picNO and (2) $[H(3\text{-picNO})_2][AuCl_4]$ showing the broad absorption for the short O-H-O hydrogen bond.

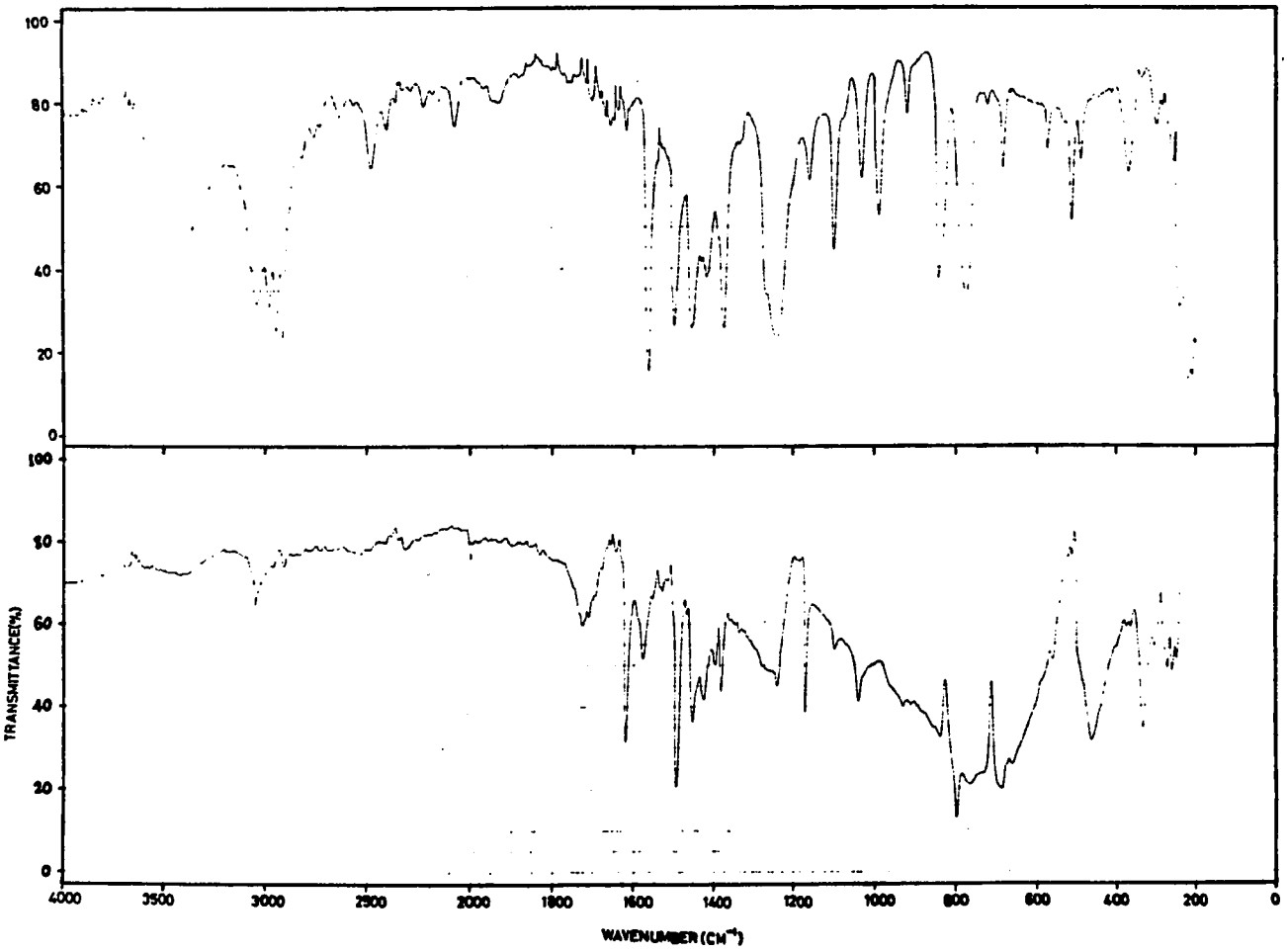


Figure 6: Infrared spectra of: (1) free 2,6-dimethylpyridine N-oxide and (2) $[H(2,6\text{-}(CH_3)_2\text{-}pyNO)_2][AuCl_4]$ showing the broad absorption for the short O-H-O hydrogen bond.

Table IV

Proton-NMR Absorptions for the Ligands and the Diadducts in Different Solvents[a].

Compound	δ_{CH_3} [b]	δ_{CH} [c]	δ_{NCH} [d]	$\delta_{O\text{-}H\text{-}O}$ [e]
$[^2H_6]$-DMSO				
[2-picNO]	2.40	7.31	8.35	-
$[H(2\text{-picNO})_2][AuCl_4]$	2.52	7.60	8.54	10.02
[3-picNO]	2.34	7.35	8.28	-
$[H(3\text{-picNO})_2][AuCl_4]$	2.35	7.44	8.28	9.82
[4-picNO]	2.61	7.58	8.45	-
$[H(4\text{-picNO})_2][AuCl_4]$	2.36	7.62	8.54	10.00
$[pNO_2\text{-pyNO}]$	-	8.40	8.58	-
$[H(pNO_2\text{-pyNO})_2][AuCl_4]$	-	8.55	8.75	11.19
[mCOOH-pyNO]	2.61	7.58	8.45	-
$[H(mCOOH\text{-pyNO})_2][AuCl_4]$	2.36	7.62	8.54	-
$[2,6\text{-}(CH_3)_2\text{-pyNO}]$	2.61	7.58	8.45	-
$[H(2,6\text{-}(CH_3)_2\text{-pyNO})_2][AuCl_4]$	2.36	7.62	8.54	-
CH_3OH				
[2-picNO]	-	7.57	8.43	-
$[H(2\text{-picNO})_2][AuCl_4]$	-	8.07	-	-
[3-picNO]	-	7.56	8.38	-
$[H(3\text{-picNO})_2][AuCl_4]$	-	7.90	8.63	-
[4-picNO]	2.58	7.52	8.37	-
$[H(4\text{-picNO})_2][AuCl_4]$	2.72	7.85	8.68	-

Continued on the next page

Table IV --(Continued)

Compound	δ_{CH_3} (b)	δ_{CH} (c)	δ_{NCH} (d)	$\delta_{O\text{-}H\text{-}O}$ (e)
CH_3CN				
[2-picNO]	-	7.47	8.37	-
$[H(2\text{-picNO})_2][AuCl_4]$	-	7.97	-	-(f)
[3-picNO]	-	7.37	8.33	-
$[H(3\text{-picNO})_2][AuCl_4]$	-	7.87	8.50	-
[4-picNO]	-	7.37	8.08	-
$[H(4\text{-picNO})_2][AuCl_4]$	-	7.93	8.13	-
DMSO				
[2-picNO]	-	7.63	8.58	-
$[H(2\text{-picNO})_2][AuCl_4]$	-	8.00	-	-
[3-picNO]	-	7.56	8.53	-
$[H(3\text{-picNO})_2][AuCl_4]$	-	8.00	8.83	-
[4-picNO]	-	7.72	8.60	-
$[H(4\text{-picNO})_2][AuCl_4]$	-	8.18	9.11	-
CH_3NO_2				
[2-picNO]	-	7.12	8.03	-
$[H(2\text{-picNO})_2][AuCl_4]$	-	7.67	8.40	-
[3-picNO]	-	7.03	7.90	-
$[H(3\text{-picNO})_2][AuCl_4]$	-	7.95	8.50	-
[4-picNO]	-	7.00	7.85	-
$[H(4\text{-picNO})_2][AuCl_4]$	-	7.60	8.40	-

(a) Absolutely moisture free $[^2H_6]$DMSO was used as a solvent. Even traces of water in the solvent obscured the resonance for the bridged protons.
(b) All resonances obscured by solvents or those which could not be detected because of rapid exchange are indicated by a dash.
(c) Center of multiplets for the phenyl protons.
(d) Center of multiplet for protons attached to the carbons next to the nitrogen.
(e) Singlet for the bridged proton.
(f) These are less soluble in the solvents than the ligands, particularly in the case of $[H(2\text{-picNO})_2][AuCl_4]$.

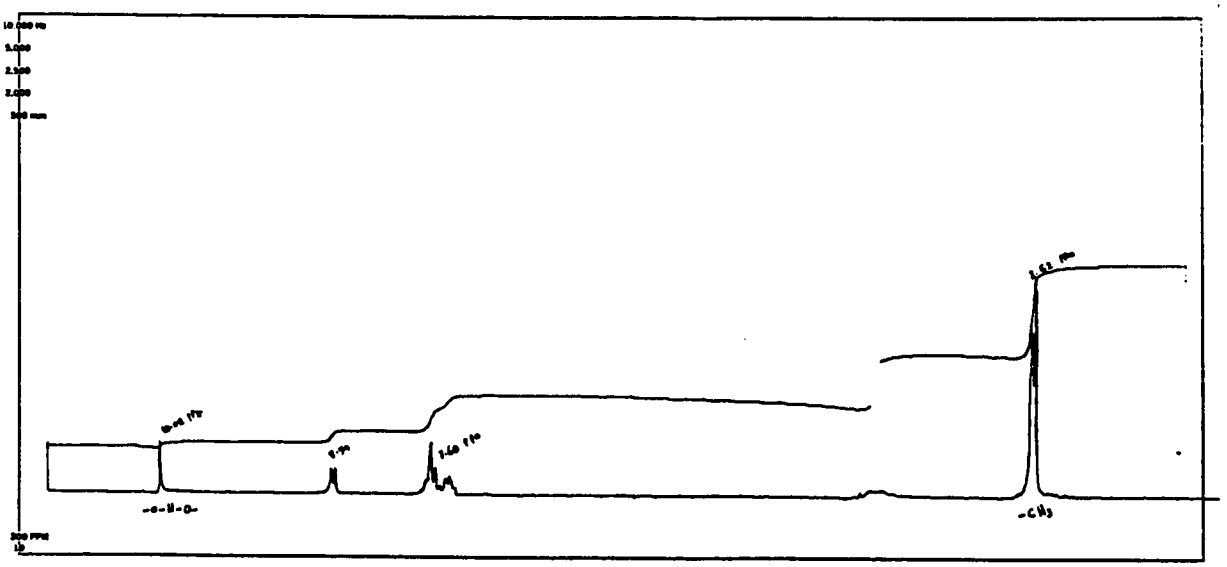


Figure 7: Proton NMR spectra of $[H(2\text{-picNO})_2][AuCl_4]$ in $[^2H_6]$-DMSO showing downfield resonance for the short hydrogen bonded proton.

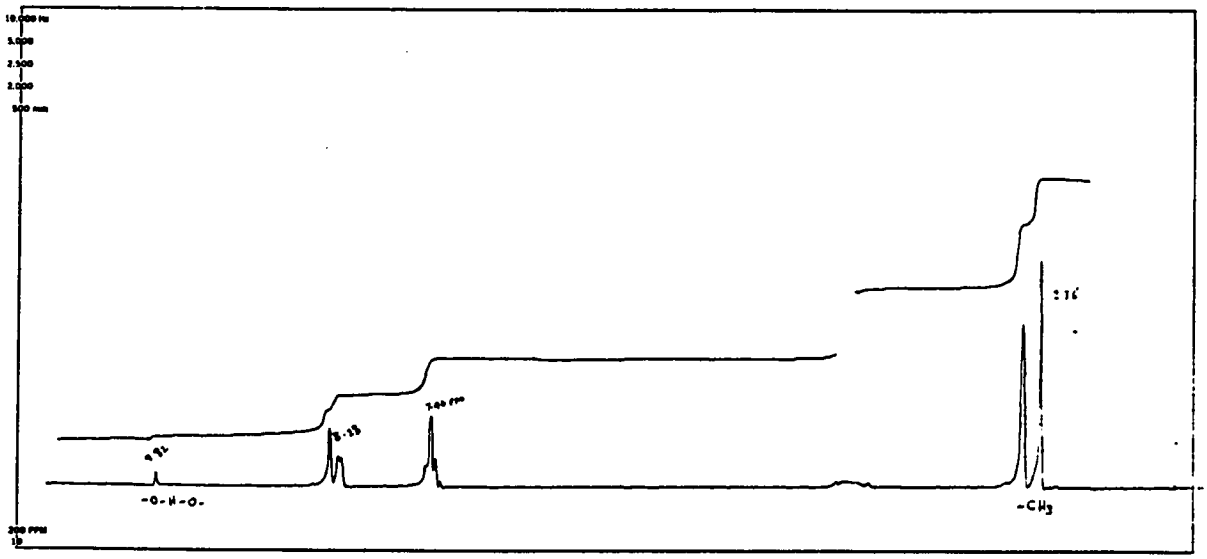


Figure 8: Proton NMR spectra of $[H(3\text{-picNO})_2][AuCl_4]$ in $[^2H_6]$-DMSO showing downfield resonance for the short hydrogen bonded proton.

2.4: Crystallographic Studies.

2.4.1: Crystal Data.

A well-formed, almost spherical light yellow crystal was mounted on a glass fiber in an arbitrary orientation. Lattice constants were obtained by the least-squares refinement of the diffraction geometry of 25 centered reflections having $\theta > 25^{o}$ using Mo-K_{α} radiation (λ= 0.71073 Å). Space group determination was done on the basis of systematic absences in the entire intensity data. The density of the crystals was measured by floatation in an appropriate solution. The density of the solvents was determined with the usual method using density bottle. Efforts were made to transform the cell to that of a higher symmetry with the lattice transformation program TRACER-II [50]. The cell parameters for all the compounds are given in Table V.

2.4.2: Intensity Data Collection and Reduction.

The x-ray intensity data were collected on an Enraf-Nonius CAD4 diffractometer controlled by a PDP8/A computer using graphite-monochromated Mo-K_{α} radiation and the ZIGZAG method in ω-2θ scan mode with a θ scan range of $(1.10+0.35\ \tan\theta)^{o}$ centered about the calculated Mo-K_{α} peak positions. The scan rate varied from 1.68 to 5.03^{o} min^{-1}. Background counts were measured for half of the total scan time by extending the scan range 25% on either side of the scan limits. Three standard reflections were monitored every 8000 s of x-ray exposure time with no indications of crystal deterioration. The crystal orientation was checked each 50 or 80 reflections. The intensities were corrected for background, Lorentz and polariza-

tion effects and equivalent and duplicate reflections were averaged to obtain the unique reflection data. Reflections with $I > 3\sigma(I)$ were used in the structure analysis and final refinement. Since the crystals were aimost perfect sphere, absorption corrections were not considered necessary. The estimated range of transmission was about 2 to 4% based on ψ scans and because of an excellent convergence in the least-squares refinement, the decision not to apply absorption corrections was considered appropriate.

2.4.3: Structure Solution and Refinement.

The coordinates for gold and chloride atoms were obtained from Patterson synthesis, or by using MULTAN [51] or by using the direct solution routine in the SHELX76 program package [52]. A difference Fourier map phased on the refined positions of heavy atoms led to the location of all carbon atoms. Several cycles of isotropic refinement followed by a few cycles of anisotropic refinement revealed the positions of most of the hydrogen atoms which agreed with the calculated positions. The hydrogen positions were refined isotropically while holding all non-hydrogen atoms at fixed positions. In the final refinement cycles a weighing scheme based on counting statistics was used. The final difference Fourier map was featureless and the largest shift in any parameter at the final stage and the highest residual peaks are listed in Tables VI, along with the details of data collection and structure solution for each compound.

Table V

Crystal Data for Gold(III) Compounds of Substituted Pyridine N-oxides.

Parameters	$[H(2\text{-picNO})_2]$-$[AuCl_4]$	$[H(3\text{-picNO})_2]$-$[AuCl_4]$	$[H(4\text{-picNO})_2]$-$[AuCl_4]$
System	Monoclinic	Triclinic	Triclinic
F. wt.	558	558	558
a (Å)	22.376(9)	6.857(4)	7.220(1)
b (Å)	9.874(6)	8.011(1)	7.516(2)
c (Å)	7.957(5)	8.797(2)	8.860(5)
$\alpha(^{o})$	90.0	105.05(2)	76.17(3)
$\beta(^{o})$	94.98(6)	66.89(3)	66.33(7)
$\gamma(^{o})$	90.0	89.39(2)	79.74(5)
λ(Å)	0.71073	0.71073	0.71073
$V(Å^3)$	1751.4(9)	425.7(4)	425.7(5)
$D_c(g\ cm^{-3})$	2.12	2.18	2.18
$D_m(g\ cm^{-3})$	2.13	2.17	2.17
Z	4	1	1
F(000)	1056	264	264
Space group	$P2_1/n$	$P\bar{1}$	$P\bar{1}$
$\mu(M_o\text{-}K_\alpha)(cm^{-1})$	89	89	89

Continued on the next page

Table V --(Continued)[a]

Parameters	$[H(pNO_2\text{-}pyNO)_2][AuCl_4]$	$[H(mCOOH\text{-}pyNO)_2][AuCl_4]$
System	Monoclinic	Triclinic
F. wt.	620	798
a(Å)	7.39(1)	7.859(2)
b(Å)	12.434(1)	8.35(2)
c(Å)	10.165(1)	10.658(7)
$\alpha(^o)$	90.0	106.59(8)
$\beta(^o)$	90.76(4)	103.97(4)
$\gamma(^o)$	90.0	100.18(7)
λ(Å)	0.71073	0.71073
$V(Å^3)$	934.2(1)	627.3(7)
$D_c(g\ cm^{-3})$	2.20	-
$D_m(g\ cm^{-3})$	2.26	-
F(000)	-	-
$\mu(M_o\text{-}K_\alpha)(cm^{-1})$	-	-

(a) Only crystal data were obtained for these two compounds. The three-dimensional structure analysis is not yet completed.

The full-matrix least-squares refinements were based on F_o, and the functions minimized were defined as $\Sigma w(|F_o| - |F_c|)^2$. Agreement factors are defined as $R=\Sigma||F_o|-|F_c||/\Sigma|F_o|$ and $R_w=[(w|F_o|-|F_c||^2/\Sigma wF_o^2)^{1/2}]$. All calculations were carried out on the University of Petroleum and Minerals IBM 3033 computer using SHELX76 or on TEXRAY230 system. Atomic scattering factors for non-hydrogen atoms were taken from Cromer and Mann [53], for H atoms from Stewart, Davidson and Simpson [54]. Anomalous dispersion correction were taken from Cromer and Liberman [55]. The atomic coordinates and thermal parameters (B_{eq}) for all atoms in each compound are given in Table VII. The anisotropic thermal parameters for non-hydrogen atoms are given in Table VIII. The observed and calculated structure factors for the three structures are included as Appendix A.

The complete structural analysis of $[H(3\text{-picNO})_2][AuCl_4]$ and of $[H(4\text{-picNO})_2][AuCl_4]$ were also carried out on TEXRAY230 system using SDP82 software [56], which became available at the final stages of work on these compounds. The electron density contour maps (Figure 15) and the overlap density functions (Figure 16) for $[H(4\text{-picNO})_2]^+$ cation were obtained using TEXRAY Graphic System of the Molecular Structure Corporation.

Table VI

Details of Data Collection and Structure Solution for $[H(2\text{-picNO})_2][AuCl_4]$.

1) Formula	$C_{12}H_{15}N_2O_2AuCl_4$
2) Method of measuring density	Floatation in Bromoform - 1,3-dibromopropane
3) Crystal shape and size, mm	Almost Spherical 0.16 x 0.15 x 0.16
4) Diffractometer used	CAD4
5) No. of Reflections used to measure lattice parameters	25
6) Absorption correction	None
7) Maximum value of 2θ (deg)	50
8) Range of hkℓ	h±k±ℓ
9) (a) standard reflections	(-1 -5 -4) (2 -5 -3) (-5 -3 -4)
(b) their intensity variation	Negligible
10) No. of reflections measured	6320
11) No. of unique reflections	3078
12) Value of R_{int}	0.008
13) No. of observed reflections	2623
14) Method used to solve structure	Direct and Heavy Atom Procedures
15) Criterion for recognizing observed reflections	$I > 3\sigma(I)$
16) Use of F or F^2 magnitudes in LS refinement	F
17) Methods of locating and refining H atoms if applicable	Difference Fourier Map and calculated positions.
18) No. of Parameters refined	208
19) Values of (a) R	0.039
and (b) R_w	0.036
20) Value of w in weighing scheme	$w=(1.8502/\delta^2(F_o)+0.001F_o^2)$
21) Ratio of max. LS shift to error	0.1
22) Max. height in final diff. Fourier	0.8 e/Å^3
23) Secondary extinction value (if used)	Not Applied
24) Source of atomic scattering factors and $\Delta f'$, $\Delta f''$ values	Reference Nos. 53-55

25) Computer programs used and their source :

XRAY	: Data Reduction and sorting Program developed at UPM.
SHELX76	: G. M. Sheldrick, University of Cambridge, England.
MULTAN78	: P. Main et. al., University of York, York, England.
ORTEPII	: Carroll K. Johnson, Oak Ridge National Laboratory, USA.
TRACERII	: Lawton, S.L., Northwestern University, U.S.A
SDP82	: B.A. Frenz & Associate, Inc. College Station, Texas & Enraf-Nonius, Delft, Holland.

Table VI --(Continued)

Details of Data Collection and Structure Solution for $[H(3\text{-picNO})_2][AuCl_4]$.

1) Formula	$C_{12}H_{15}N_2O_2AuCl_4$
2) Method of measuring density	Floatation in Bromoform - 1,3-dibromopropane
3) Crystal shape and size, mm	Almost Spherical 0.14 x 0.15 x 0.14
4) Diffractometer used	CAD4
5) Reflections used to measure lattice parameters	25
6) Absorption correction	None
7) Maximum value of 2θ (deg)	60^o
8) Range of hkℓ	h±k±ℓ
9) (a) standard reflections	(0 4 -1) (0 4 0) (1 4 0)
(b) their intensity variation	Negligible
10) No. of reflections measured	2568
11) No. of unique reflections	2479
12) Value of R_{int}	0.008
13) No. of observed reflections	2334
14) Method used to solve structure	Direct and Heavy Atom Procedures
15) Criterion for recognizing observed reflections	$I > 3\sigma(I)$
16) Use of F or F^2 magnitudes in LS refinement	F
17) Methods of locating and refining H atoms if applicable	Difference Fourier Map and calculated positions.
18) No. of Parameters refined	105
19) Values of (a) R	0.063
and (b) R_w	0.066
20) Value of w in weighing scheme	unit weights
21) Ratio of max. LS shift to error	0.181
22) Max. height in final diff. Fourier	1.2 e/Å^3
23) Secondary extinction value (if used)	Not Applied
24) Source of atomic scattering factors and $\Delta f'$, $\Delta f''$ values	Reference Nos. 53-55

25) Computer programs used and their source : As on previous page

Table VI --(Continued)

Details of Data Collection and Structure Solution for $[H(4\text{-picNO})_2][AuCl_4]$.

1) Formula	$C_{12}H_{15}N_2O_2AuCl_4$
2) Method of measuring density	Floatation in Bromoform - 1,3-dibromopropane
3) Crystal shape and size, mm	Almost Spherical 0.14 x 0.15 x 0.14
4) Diffractometer used	CAD4
5) Reflections used to measure lattice parameters	25
6) Absorption correction	None
7) Maximum value of 2θ (deg)	60^o
8) Range of hkℓ	h±k±ℓ
9) (a) standard reflections	(0 3 3) (1 -2 2) (1 2 3)
(b) their intensity variation	Negligible
10) No. of reflections measured	2751
11) No. of unique reflections	2481
12) Value of R_{int}	0.017
13) No. of observed reflections	1388
14) Method used to solve structure	Direct and Heavy Atom Procedures
15) Criterion for recognizing observed reflections	$I > 3\sigma(I)$
16) Use of F or F^2 magnitudes in LS refinement	F
17) Methods of locating and refining H atoms if applicable	Difference Fourier Map and calculated positions.
18) No. of Parameters refined	97
19) Values of (a) R	0.067
and (b) R_w	0.073
20) Value of w in weighing scheme	$w=(1.0/(\delta^2(F_o)+0.027\ \|F_o\|^2)$
21) Ratio of max. LS shift to error	0.181
22) Max. height in final diff. Fourier	1.2 e/Å^3
23) Secondary extinction value (if used)	Not Applied
24) Source of atomic scattering factors and $\Delta f'$, $\Delta f''$ values	Reference Nos. 53-55
25) Computer programs used and their source	: As on previous page

Table VII

Positional and Thermal Parameters for $[H(2\text{-PicNO})_2][AuCl_4]$.

Atom	x/a	y/b	z/c	B_{eq} Å^2
Au	0.3792(0)	0.3135(0)	0.2682(0)	3.16
Cl(1)	0.4415(1)	0.1346(2)	0.3291(3)	4.85
Cl(2)	0.3055(1)	0.2047(2)	0.3901(4)	5.74
Cl(3)	0.3152(1)	0.4885(2)	0.2092(3)	5.44
Cl(4)	0.4541(1)	0.4263(3)	0.1531(3)	5.89
O(1)	0.8280(3)	0.3365(5)	0.4232(9)	4.97
N(2)	0.8511(3)	0.4605(6)	0.4518(8)	3.59
C(3)	0.9050(3)	0.4886(8)	0.3927(9)	3.40
C(4)	0.9292(4)	0.6131(9)	0.426(1)	4.17
C(5)	0.8987(5)	0.7103(9)	0.511(1)	5.07
C(6)	0.8437(5)	0.6771(9)	0.568(1)	5.27
C(7)	0.8209(4)	0.5494(9)	0.536(1)	4.60
C(8)	0.9341(4)	0.378(1)	0.299(1)	5.02
O(9)	0.7338(3)	0.3705(9)	0.2624(9)	7.06
N(10)	0.6886(3)	0.3221(7)	0.3464(9)	4.57
C(11)	0.6392(5)	0.3930(9)	0.351(1)	4.86
C(12)	0.5933(5)	0.339(1)	0.434(1)	5.73
C(13)	0.5989(5)	0.218(1)	0.505(1)	6.59
C(14)	0.6517(6)	0.141(1)	0.494(2)	7.03
C(15)	0.6969(5)	0.192(1)	0.416(1)	5.72
C(16)	0.6350(7)	0.525(1)	0.271(2)	8.48
OHO	0.775(5)	0.311(8)	0.32 (1)	0.95
HC(4)	0.9704(4)	0.6620(9)	0.399(1)	0.95
HC(5)	0.9266(5)	0.7998(9)	0.516(1)	0.95
HC(6)	0.8291(5)	0.7664(9)	0.632(1)	0.95
HC(7)	0.7881(4)	0.6011(9)	0.605(1)	0.95
H1C(8)	0.9763(4)	0.414(1)	0.260(1)	0.95
H2C(8)	0.9050(4)	0.350(1)	0.189(1)	0.95
H3C(8)	0.9420(4)	0.292(1)	0.380(1)	0.95
HC(12)	0.5490(5)	0.373(1)	0.458(1)	0.95
HC(13)	0.5707(5)	0.156(1)	0.577(1)	0.95
HC(14)	0.6447(6)	0.046(1)	0.557(2)	0.95
HC(15)	0.7029(5)	0.087(1)	0.451(1)	0.95
H1C(16)	0.5916(7)	0.569(1)	0.287(2)	0.95
H2C(16)	0.6405(7)	0.515(1)	0.138(2)	0.95
H3C(16)	0.6698(7)	0.590(1)	0.328(2)	0.95

Continued on the next page

Table VII--(continued)

Positional and Thermal Parameters for $[H(3\text{-PicNO})_2][AuCl_4]$.

Atom	x/a	y/b	z/c	B_{eq} $Å^2$
Au	0.0000(0)	0.0000(0)	0.0000(0)	2.72
Cl(1)	0.2222(7)	-0.0535(5)	-1.2836(4)	4.47
Cl(2)	-0.0258(7)	0.2921(4)	-0.9723(5)	4.66
O(1)	0.351(1)	0.006(1)	-0.869(1)	5.26
N(2)	0.321(1)	0.160(1)	-0.748(1)	3.42
C(3)	0.372(2)	0.302(1)	-0.801(1)	3.74
C(4)	0.341(2)	0.463(1)	-0.677(1)	3.51
C(5)	0.249(2)	0.467(1)	-0.504(1)	3.54
C(6)	0.197(2)	0.317(1)	-0.455(1)	3.94
C(7)	0.235(2)	0.161(1)	-0.582(1)	4.02
C(8)	0.400(2)	0.620(1)	-0.741(2)	5.58
OHO	0.303(1)	-0.096(1)	-0.808(1)	0.95
HC(3)	0.518(2)	-0.024(1)	-0.958(1)	0.95
HC(5)	0.257(2)	0.017(1)	-0.941(1)	0.95
HC(6)	0.129(2)	0.322(1)	-0.320(1)	0.95
HC(7)	0.196(2)	0.042(1)	-0.548(1)	0.95
H1C(8)	0.367(2)	0.734(1)	-0.633(2)	0.95
H2C(8)	0.307(2)	0.639(1)	-0.811(2)	0.95
H3C(8)	0.568(2)	0.600(1)	-0.826(2)	0.95

Continued on the next page

Table VII--(continued)

Positional and Thermal Parameters for $[H(4\text{-PicNO})_2][AuCl_4]$[a]

Atom	x/a	y/b	z/c	B_{eq} $Å^2$(b)
Au	0.0	0.0	0.0	2.50
Cl(1)	0.0443(7)	0.2943(7)	0.1341(6)	3.94
Cl(2)	0.0302(8)	-0.1105(7)	-0.2275(5)	4.16
O(1)	0.477(2)	0.036(2)	0.866(2)	3.99
N(2)	0.522(2)	0.210(2)	0.797(2)	3.27
C(3)	0.421(3)	0.350(3)	0.872(2)	3.67
C(4)	0.468(3)	0.526(2)	0.798(2)	3.58
C(5)	0.617(2)	0.564(2)	0.642(2)	2.93
C(6)	0.718(3)	0.415(2)	0.564(2)	3.01
C(7)	0.670(3)	0.241(2)	0.642(2)	3.27
C(8)	0.674(4)	0.758(3)	0.564(3)	4.50
OHO	0.559(0)	1.036(0)	0.0	0.95
HC(3)	0.300(3)	0.324(3)	0.994(2)	0.95
HC(4)	0.386(3)	0.637(2)	0.863(2)	0.95
HC(6)	0.836(3)	0.438(2)	0.440(2)	0.95
HC(7)	0.750(3)	0.127(2)	0.580(2)	0.95
H1C(8)	0.794(4)	0.758(3)	0.442(3)	0.95
H2C(8)	0.726(4)	0.808(3)	0.642(3)	0.95
H3C(8)	0.544(4)	0.845(3)	0.550(3)	0.95

(a) Number in parentheses in this and all subsequent tables represent estimated standard deviations in the last digit.

(b) The B_{eq} values were calculated as $B_{eq}=8\pi^2U_{eq}$ and U_{eq}=1/3 trace U

Table VIII

Anisotropic Thermal Parameters for $[H(2\text{-PicNO})_2][AuCl_4]$.

Atom	U11	U22	U33	U23	U13	U12
Au	0.0374(2)	0.0392(2)	0.0439(2)	0.0012(1)	0.0064(1)	-0.0011(1)
Cl(1)	0.051(1)	0.061(1)	0.075(1)	0.017(1)	0.018(1)	0.014(1)
Cl(2)	0.053(1)	0.057(1)	0.114(2)	0.016(1)	0.036(1)	-0.000(1)
Cl(3)	0.064(1)	0.047(1)	0.096(2)	0.013(1)	0.010(1)	0.011(1)
Cl(4)	0.055(1)	0.075(2)	0.096(2)	0.032(1)	0.018(1)	-0.010(1)
O(1)	0.053(4)	0.046(3)	0.100(5)	-0.004(3)	0.006(3)	-0.016(3)
N(2)	0.041(3)	0.043(3)	0.053(4)	0.003(3)	0.004(3)	-0.003(3)
C(3)	0.036(4)	0.048(4)	0.045(4)	-0.000(3)	0.000(3)	0.001(3)
C(4)	0.045(4)	0.061(5)	0.052(5)	0.006(4)	0.000(4)	-0.009(4)
C(5)	0.075(6)	0.048(5)	0.068(6)	0.007(4)	-0.007(5)	-0.005(4)
C(6)	0.082(7)	0.052(5)	0.067(6)	-0.013(4)	0.009(5)	0.011(5)
C(7)	0.051(4)	0.061(5)	0.064(5)	-0.000(4)	0.013(4)	0.006(4)
C(8)	0.054(5)	0.070(6)	0.067(6)	-0.015(5)	0.009(4)	0.007(4)
O(9)	0.057(4)	0.133(6)	0.077(5)	0.024(4)	-0.002(4)	-0.031(4)
N(10)	0.051(4)	0.068(5)	0.053(4)	-0.001(3)	-0.006(3)	-0.013(4)
C(11)	0.079(6)	0.050(5)	0.053(5)	0.005(4)	-0.014(4)	0.000(4)
C(12)	0.061(6)	0.091(8)	0.065(6)	-0.009(5)	0.001(5)	-0.003(5)
C(13)	0.077(8)	0.113(9)	0.060(6)	0.010(6)	0.001(5)	-0.023(7)
C(14)	0.105(0)	0.075(7)	0.083(8)	0.028(6)	-0.022(7)	-0.020(7)
C(15)	0.069(6)	0.061(6)	0.084(7)	0.008(5)	-0.016(5)	-0.007(5)
C(16)	0.16 (1)	0.056(7)	0.096(0)	0.011(6)	-0.032(9)	-0.005(8)

Continued on the next page

Table VIII--(Continued)

Anisotropic Thermal Parameters for $[H(3\text{-}PicNO)_2][AuCl_4]$.

Atom	U11	U22	U33	U23	U13	U12
Au	0.0454(4)	0.0251(3)	0.0264(3)	-0.0008(2)	-0.0123(3)	0.0009(2)
Cl(1)	0.072(2)	0.048(1)	0.031(1)	0.003(1)	-0.006(1)	0.005(1)
Cl(2)	0.085(2)	0.028(1)	0.049(1)	0.004(1)	-0.019(1)	0.001(1)
O(1)	0.083(2)	0.037(2)	0.064(2)	-0.016(2)	-0.025(2)	-0.005(2)
N(2)	0.048(2)	0.032(2)	0.041(2)	-0.006(2)	-0.015(2)	-0.001(2)
C(3)	0.052(2)	0.040(2)	0.038(2)	0.002(2)	-0.014(2)	0.001(2)
C(4)	0.047(2)	0.038(2)	0.041(2)	0.001(2)	-0.017(2)	0.002(2)
C(5)	0.048(2)	0.044(2)	0.035(2)	-0.008(2)	-0.013(2)	0.005(2)
C(6)	0.052(2)	0.056(2)	0.032(2)	0.002(2)	-0.014(2)	0.002(2)
C(7)	0.049(2)	0.043(2)	0.046(2)	0.009(2)	-0.014(2)	-0.003(2)
C(8)	0.089(2)	0.039(2)	0.060(2)	0.010(2)	-0.021(2)	-0.005(2)

Continued on the next page

Table VIII--(continued)

Anisotropic Thermal Parameters for $[H(4\text{-PicNO})_2][AuCl_4]$[(a)].

Atom	U11	U22	U33	U23	U13	U12
Au	0.0209(4)	0.0361(6)	0.0353(6)	-0.0081(4)	-0.0085(3)	-0.0013(3)
Cl(1)	0.052(2)	0.046(2)	0.043(2)	-0.004(2)	-0.015(2)	0.002(2)
Cl(2)	0.062(3)	0.056(3)	0.036(2)	-0.014(2)	-0.012(2)	-0.006(2)
O(1)	0.065(9)	0.042(7)	0.050(7)	0.001(6)	-0.024(6)	-0.022(6)
N(2)	0.044(7)	0.041(8)	0.034(7)	-0.003(6)	-0.011(6)	-0.013(6)
C(3)	0.036(8)	0.06(1)	0.035(8)	-0.019(8)	-0.006(6)	0.004(8)
C(4)	0.06(1)	0.028(9)	0.05(1)	-0.016(8)	-0.021(8)	-0.000(7)
C(5)	0.036(8)	0.036(9)	0.042(8)	-0.005(7)	-0.009(6)	-0.010(6)
C(6)	0.050(9)	0.041(9)	0.016(6)	-0.003(6)	-0.001(6)	-0.011(7)
C(7)	0.043(9)	0.035(9)	0.045(9)	-0.012(7)	-0.012(7)	0.000(7)
C(8)	0.07(1)	0.04(1)	0.06(1)	0.000(9)	-0.02(1)	-0.02(1)

(a) The temperature factors are of the form:

$$\exp[-2\pi^2(U_{11}h^2a^{*2} + U_{22}k^2b^{*2} + U_{33}\ell^2c^{*2} + 2U_{12}hka^*b^* + 2U_{13}h\ell ac^* + 2U_{23}k\ell b^*c^*)]$$

CHAPTER THREE

3. RESULTS AND DISCUSSION

3.1: General Formulation of the Compounds.

In all reactions with $HAuCl_4$ or $NaAuCl_4$, the heterocyclic N-oxides did not replace the chloride from the primary coordination sphere of the gold(III) atom and in all cases only products of the general formula $[H(R\text{-picNO})_2][AuCl_4]$ (where R = 2-Me, 3-Me and 4-Me, p-NO_2, m-COOH and 2,6-$(CH_3)_2$) were obtained. No complexes of the general formula $H[(R\text{-pyNO})_2AuCl_4]$ with monodentate N-oxide or any other species in which any of the chloride was replaced by the N-oxide, were formed under the present preparative conditions irrespective of the N-oxide:metal ratio or the basicity of the N-oxide. Thus, for the formation of crystalline salts of the hydrogen-bonded dimeric cations of aromatic N-oxides $[AuCl_4]^-$ is probably the most suitable anion.

3.2: Electronic Absorption Spectra.

The ultraviolet-visible spectral data in the range 190-750 nm for the free N-oxides and their compounds with gold(III) chloride are given in Table II. Three representative spectra are shown in Figures 1 - 3. All the free ligands (i.e heterocyclic N-oxides) have two relatively intensive bands around 215 and 260 nm in the u.v. region with molar absorptivities of ca. 10^4 or greater. Both bands in the free ligands tail towards the visible region without any peak appearing in this region. A methanolic solution of $HAuCl_4$ has a medium intensity absorption centred at 320 nm and a very

weak broad band with λ_{max} at ca. 410 nm [57]. In the gold(III) chloride compounds, the higher energy band (i.e 215 nm band) is further intensified, with the appearance of a shoulder around 225 nm between the two u.v. bands and a broad absorption of fairly high molar absorptivity around 315 nm, indicative of the $[AuCl_4]^-$ anion [57]. The presence of the ligand as well as $[AuCl_4]^-$ bands was used as indication of product formation in solution. The high value of extinction coefficients for all the bands (particularly for the one at 315 nm) makes these heterocyclic N-oxides suitable reagents for extraction as well as photometric determination of gold. The selectivity for extraction of gold and the interference of other ions are yet to be examined.

3.3: Vibrational Spectra of Compounds with Short-hydrogen Bond.

The free hydroxyl group has a stretching frequency near 3400 cm^{-1}, as observed in the gases or in inert solvents. Striking changes are observed when hydrogen bonding occurs, whether in gases, solutions or crystals. The absorption peaks move to lower frequencies and become much broadened, implying a large increase of integrated intensities. Over a range of weak (or large) O-H..O bonds there is a good correlation between the overall length and the peak frequency, which may fall as low as 2,000 cm^{-1}.

However, with "short hydrogen bonded" systems of the type $[BHB]^+$ the spectra become much more complicated especially when the two B-units in the above formula are equivalent [58]. The O-H stretching band does not appear in the region above 2,000 cm^{-1}, instead, there is a general

absorption over several hundred cm^{-1}, culminating around 1050 cm^{-1}. Various peaks are superimposed on this wide background absorption which is often overlaid with a number of maxima corresponding to the free ligands. Such spectra have been classified as Type (ii) by Hadzi [59], who termed the wide absorption as the "D band".

All significant absorptions in the infrared region for the free N-oxides and their gold(III) chloride compounds are listed in Table III. Three representative spectra are shown in Figures 4-6. An intense and broad region of absorptions extending over the range 650-1050 cm^{-1} was observed in all compounds clearly indicating the existence of O-H-O short hydrogen bond [26,60]. Furthermore, the absence of any absorptions in the hydroxyl region (i.e around 3400 cm^{-1}) in perfectly anhydrous conditions indicates a short (or strong) O-H-O hydrogen bond rather than the O-H stretching mode in a long (or weak) O-H..O type bond. A weak and broad band around 3400 cm^{-1} observed in some compounds is due to moisture because this band disappeared or diminished when the compound was carefully dried.

In coordination compounds with monodentate pyNO or its derivatives, a prominent ν(N-O) stretching band observed around 1250 cm^{-1} in the free base, is shifted about 40 cm^{-1} toward lower frequency on complexation, suggesting metal-oxygen bond formation [61]. In the protonated dimeric species, although the ν(N-O) frequency (Table III) is somewhat obscured by the tail of the broad and intense 'D band', a peak around 1210 cm^{-1} in the products corresponds to the ν(N-O) absorption observed at 1250 cm^{-1} as an intense and sharp peak in the free N-oxides.

The Au-Cl stretching absorptions in $[AuCl_4]^-$ below 600 cm^{-1} are also obscured by the ligand absorptions in this region. Therefore, no band assignments were attempted.

3.4: Proton-NMR Spectra.

Hydrogen bonding decreases the electron density around the proton and moves the proton n.m.r. absorption to lower field. Thus, the proton-n.m.r. chemical shifts, are very useful for the purpose of identification of short hydrogen bonds. The chemical shift values for the bridged proton should be approximately related to the shielding of the proton by the N=O group which in turn may be attributed to the inductive influence of the substituents on the aromatic ring of the N-oxide. A reasonable correlation should exist between the O---O separation and the chemical shifts of the bridged proton. Proton n.m.r. spectra (Table IV) in various solvents such as $[^2H_6]$dmso, CH_3OH, CH_3CN, DMSO and CH_3NO_2, revealed all non-equivalent proton resonances with expected multiplicities and correct integrated intensities except for the H-bonded proton resonance which could be detected only for four compounds in absolutely anhydrous $[^2H_6]$dmso. Efforts to detect bridged-proton signals, even in freshly prepared highly concentrated solution of the gold(III) compounds were not successful except for the four cases above. The failure to observe this signal is due to the traces of water in the solvent (or moisture in the compound) which would effectively eliminate the signal by rapid exchange [62]. The n.m.r spectra of two of the four cases in which H-bonded proton signals were clear, are shown in Figures 7 and 8. The down-field chemical shift for the bridged proton with methyl substituent at 2-, 3- and 4-positions are 10.00, 9.82

and 10.0 p.p.m relative to TMS, respectively. An electron-withdrawing $-NO_2$ group at 4-position resulted in further deshielding of the proton to give δ value of 11.19 p.p.m. The identical values for the ortho- and para-substituents indicate similar inductive effects on the pyNO ring by such substituent. This is expected from enhanced contribution of a similar set of resonance structures resulting from an electron-donating substituent (i.e methyl group) at the 2- or 4-positions [8]. The δ value of about 10.0 p.p.m for the resonance of the bridged proton in these cationic diadducts are significantly less than δ of 18.5 p.p.m observed for the intramolecular short-hydrogen bonded proton in vic-dioximates or in neutral chelated complexes of α-amine dioximes extensively studied by Hussain and Schlemper [37-42]. Furthermore, in the chelated structures the n.m.r. signals for the bridged proton could be easily detected in $[^2H_6]$dmso, probably because of the steric shielding of the bond by the ligand against any rapid exchange of the bridged proton with the solvent. The δ value for the bridged proton in the carboxylic acid dimers are found as far downfield as about δ 13.2 to δ 10.0 p.p.m. in non-polar solvents [63] which is approximately in the same range observed for the aromatic N-oxide diadducts. Ziegler reported [32] a downfield δ value of 17.45 p.p.m for the $[H(dma)_2][AuCl_4]$.

3.5: Crystallographic Results.

Although the spectroscopic results indicate that all the gold(III) chloride compounds studied here consist of dimeric cations of the type $[(BHB)]^+$ (B = substituted aromatic N-oxides) stabilized by the 4-coordinate planar $[AuCl_4]^-$ anion, yet the presence or absence of any strong or weak interactions between the N-oxides and the gold atom

through oxygen of the N=O group cannot be clearly established or ruled out on the basis of spectroscopic measurements. Erroneous conclusions were drawn by earlier workers [32-33] about the stereochemistry of gold in $[H(dma)_2][AuCl_4]$ and $[H(pyNO)_2][AuCl_4]$ on the basis of i.r. and ^{1}H-n.m.r results, still those were valid conclusions because an uncommon distorted octahedral environment of gold(III) can not be discarded on the basis of spectral data alone. Thus, the crystallographic structure determination becomes necessary to provide unequivocal information about various structural possibilities.

The complete three-dimensional single crystal structure analysis of three compounds, namely $[H(R\text{-}pyNO)_2][AuCl_4]$ (R = 2-CH_3, 3-CH_3 and 4-CH_3), were performed and only preliminary crystal data were obtained on $[H(pNO_2\text{-}pyNO)_2][AuCl_4]$ and $[H(mCOOH\text{-}pyNO)_2][AuCl_4]$. The $[H(2\text{-}picNO)_2][AuCl_4]$ is crystallographically different from its 3- and 4-picNO analogs due to its symmetry independent O-H-O bond, which is very rare [20] in dimeric cations (see later).

3.5.1: Structure of $[H(2\text{-}picNO)_2]^+$ Cation in $[H(2\text{-}picNO)_2][AuCl_4]$.

In contrast to all known examples (Table IX) the $[H(2\text{-}picNO)_2][AuCl_4]$ crystallizes with four formula units per unit cell in a monoclinic space group $P2_1/n$ (order four) exhibiting a Speakman's pseudo-Type A structure [20,64] with symmetry-free short hydrogen bond rendering the cation free to assume a conformation not obscured by symmetry. One each of a well-defined, discrete dimeric cation, $[H(2\text{-}picNO)_2]^+$, and $[AuCl_4]^-$ anion constitute an asymmetric unit. The crystallographic packing of the ions in the

unit cell is shown in Figure 9. There being four formula units in the cell, the implications of the space group are that the cation and anion both be on general positions. This makes the structure unique because it differs from the known structures of similar dimeric salts [21,24] and also from the structure of Dunlop's salt [26] in which $[H(2\text{-picNO})_2]^+$ lies across a centre of symmetry and [ClHCl] across a twofold axis. There are no unusual non-bonding interactions among the ions and the packing in the crystal lattice is primarily electrostatic in nature.

Table IX. **Comparison of Crystallographic Symmetry and Short Hydrogen Bond in Some Dimeric Cations.**

Compound	Space Group	F. units per cell	symmetry of cation	O---O distance	Ref.
$[H(Ph_3PO)_2][AuCl_4]$	C2/c	4	$\bar{1}$	2.39	65
$[H(PyNO)_2][AuCl_4]$	$P\bar{1}$	1	$\bar{1}$	2.41(1)	24
$[H(dma)_2][AuCl_4]$	$P2_1/c$	2	$\bar{1}$	2.46(5)	21
				2.43(2)	
$[H(H_2O)_2][Au(CN)_2]$	$P2_1/c$	2	$\bar{1}$	2.47(2)	66
$[H(H_2O).2H_2O][AuCl_4]$	C2/m	2	2/m	2.57(1)	67
$[H(CH_3)_2PyNO]ClO_4$	Cccm	4	2/m	2.345(13)	27
$[H(2\text{-picNO})_2]Cl.3H_2O$	Pccn	4	$\bar{1}$	2.414(3)	26
$[H(Ph_3AsO)_2]Hg_2Br_6]$	C2/c	4	None	2.40(3)	68
$[H(2\text{-PicNO})_2][AuCl_4]$	$P2_1/n$	4	None	2.393(6)	-

The atom-numbering system, corresponding to Table VII, is shown in Figure 10. The principal bond lengths and angles including some intermolecular non-bonded data, are listed in Table XI. The two 2-picNO moieties in

the cation are crystallographically non-equivalent but their dimensions hardly differ. Because of the absence of symmetry in the present compound, nearly twice as many dimensions need to be listed. The average values of CH_3-C, C-C and C-N bonds and angles involving these bonds are in agreement in the two 2-picNO moieties as well as with the corresponding values in other similar structures. The average N-O distance of 1.345(8)Å is slightly shorter than the corresponding distance of 1.362(8)Å in $[H(pyNO)_2][AuCl_4]$ and of 1.358(2)Å in Dunlop's salt [26].

Table X. Least-square Planes and Dihedral Angles of $[H(2\text{-picNO})_2][AuCl_4]$.

Plane 1 : $AuCl_4^-$ Anion

$-0.218X - 0.412Y - 0.885Z + 4.977 = 0$

Au	0.0110(3)		
Cl(1)	0.017(2)	Cl(3)	0.017(2)
Cl(2)	-0.023(3)	Cl(4)	-0.022(3)

Plane 2 : 2-picNO (Molecule I)

$-0.392X + 0.328Y - 0.860Z + 8.927 = 0$

O(1)	-0.010(7)	C(5)	0.005(10)
N(2)	0.001(6)	C(6)	0.004(10)
C(3)	0.006(7)	C(7)	0.002(9)
C(4)	-0.020(8)	C(8)	0.009(9)

Plane 3 : 2-picNO (Molecule II)

$-0.312X - 0.420Y - 0.853Z + 8.382 = 0$

O(9)	0.013(7)	C(13)	-0.005(11)
N(10)	-0.020(7)	C(14)	0.019(12)
C(11)	-0.000(9)	C(15)	-0.011(11)
C(12)	0.000(11)	C(16)	0.004(13)

Dihedral Angles

Plane 1	Plane 2	Angle (°)
1	2	44.7
1	3	5.7
2	3	44.1

Table XI

Selected Bond Length (Å) and Angles (°) in $[H(2\text{-picNO})_2][AuCl_4]$.

(a) Bonding distances

Au-Cl(1)	2.277(2)	Au-Cl(2)	2.256(2)
Au-Cl(3)	2.268(2)	Au-Cl(4)	2.271(2)
O(1)-N(2)	1.341(7)	O(9)-N(10)	1.311(12)
N(2)-C(3)	1.361(9)	N(10)-C(11)	1.31(1)
N(2)-C(7)	1.36(2)	N(10)-C(15)	1.40(1)
C(3)-C(4)	1.36(1)	C(11)-C(12)	1.37(1)
C(4)-C(5)	1.39(1)	C(12)-C(13)	1.32 (2)
C(5)-C(6)	1.39(1)	C(13)-C(14)	1.42(2)
C(6)-C(7)	1.36(3)	C(14)-C(15)	1.33 (1)
C(3)-C(8)	1.50(1)	C(11)-C(16)	1.45(1)
OHO-O(1)	1.42(11)	OHO-O(9)	1.15(10)

(b) Bonding angles

Cl(1)-Au-Cl(2)	89.8(1)	Cl(2)-Au-Cl(3)	88.8(1)
Cl(3)-Au-Cl(4)	91.0(1)	Cl(4)-Au-Cl(1)	90.4(1)
C(5)-C(4)-C(3)	121.2(8)	C(6)-C(5)-C(4)	118.9(8)
C(4)-C(3)-N(2)	117.8(2)	C(8)-C(3)-C(4)	124.8(7)
C(7)-N(2)-O(1)	119.0(7)	C(8)-C(3)-N(2)	117.4(7)
C(7)-N(2)-C(3)	123.1(7)	C(7)-C(6)-C(5)	118.6(8)
C(3)-N(2)-O(1)	117.9(6)	C(6)-C(7)-N(2)	120.3(8)
O(9)-N(10)-C(11)	119.7(8)	O(9)-N(10)-C(15)	116.2(8)
C(11)-N(10)-C(15)	124.0(8)	N(10)-C(11)-C(12)	118.3(8)
C(16)-C(11)-N(10)	119.0(1)	C(16)-C(11)-C(12)	122.0(1)
C(11)-C(12)-C(13)	120.5(1.0)	C(12)-C(13)-C(14)	120.6(1.1)
C(13)-C(14)-C(15)	119.5(1.1)	C(14)-C(15)-C(16)	116.9(1.0)

(c) Non-bonding distances and angles

O(1)---O(9)	3.393(6)	O(1)---OHO---O(9)	137(7)
Cl(1)---Cl(2)	3.200(3)	Cl(1)---Au---Cl(1)	179.96
Cl(2)---Cl(3)	3.166(4)	Cl(2)---Au---Cl(2)	180.00
Cl(3)---Cl(4)	3.238(4)		
Cl(4)---Cl(1)	3.226(4)		
O(1)---O(1)	2.393(6)		
Au---O(1)	3.420(3)		

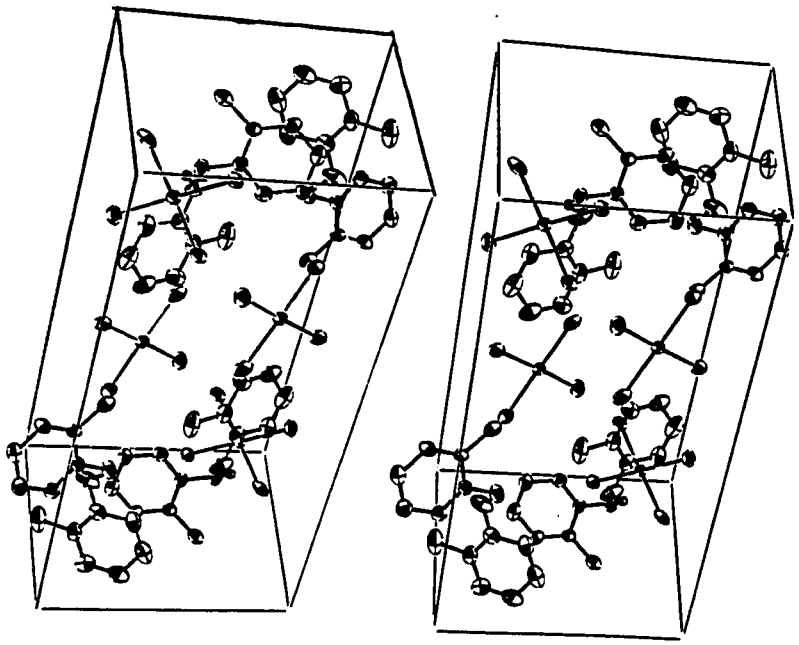
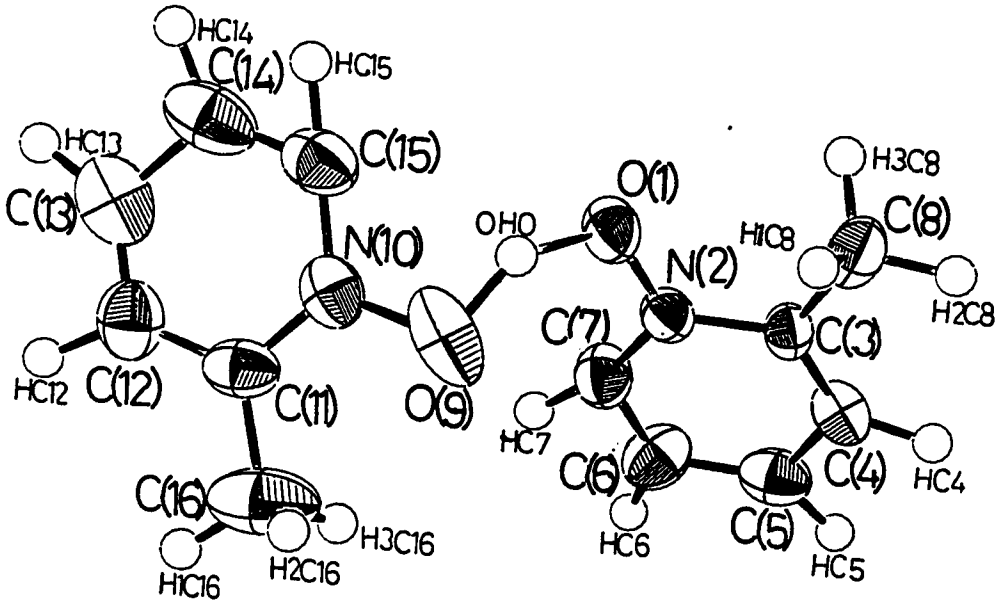
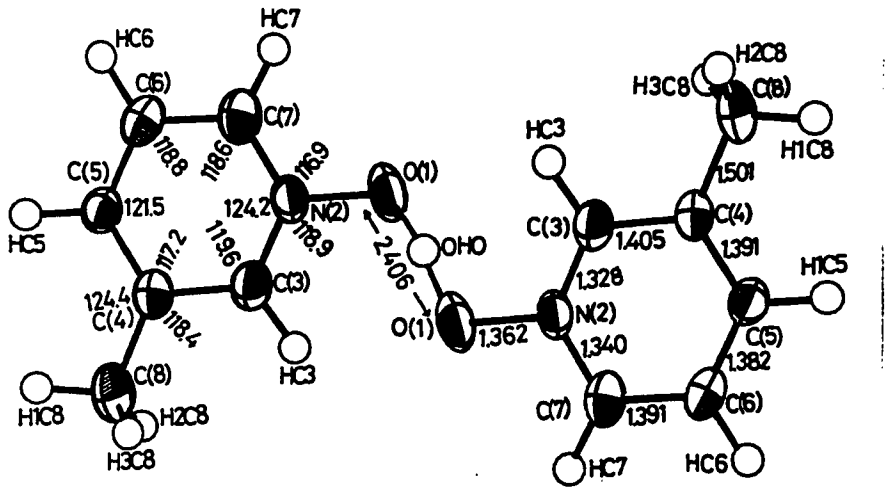


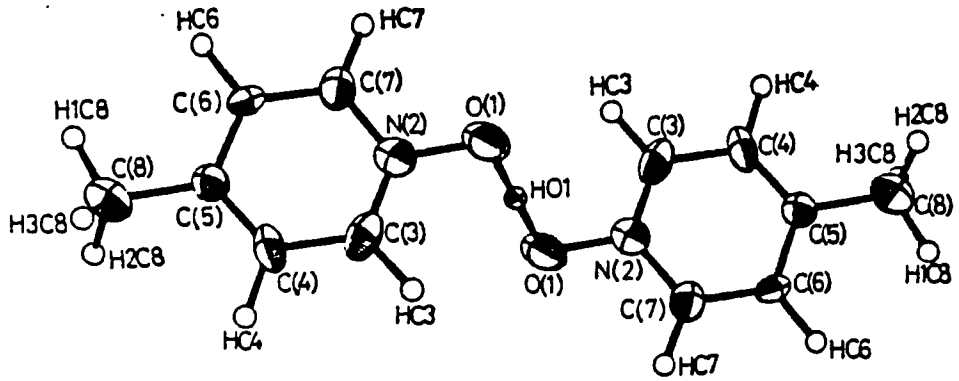
Figure 9: Stereoscopic view showing packing of $[AuCl_4]^-$ and $[H(2\text{-picNO})_2]^+$ ions in the monoclinic unit cell.



(a)



(b)



(c)

Figure 10: ORTEP diagram (45 % probability ellipsoids) showing relative orientation of the diadducts: (a) $[H(2\text{-picNO})_2]^+$ (b) $[H(3\text{-picNO})_2]^+$ and (c) $[H(4\text{-picNO})_2]^+$

The least-squares plane defined by the oxygen atom, methyl carbon and the six atoms of the pyridine ring for the two 2-picNO moieties are given in Table X. Deviations from these planes are very small and the dihedral angle between the normals to the two rings is 44.1°. Similar nonlinear arrangement having a dihedral angle of 86.6° was observed [29] for the two planar pyridine rings in $[H(C_5H_5)_2]^+$ cation in $[H(C_6H_5)_2][nBr_{3/2}Cl_{3/2}(C_5H_5N)]$ salt. When no symmetry constraints are involved, it appears that two rings in the cations adopts an orientation dictated by packing considerations in the unit cell which are influenced by the steric requirements of the base and the large size of the anion. A change in the anion or the base with different steric requirements may result in an altogether different relative arrangement of the base moieties in the dimeric cation [26].

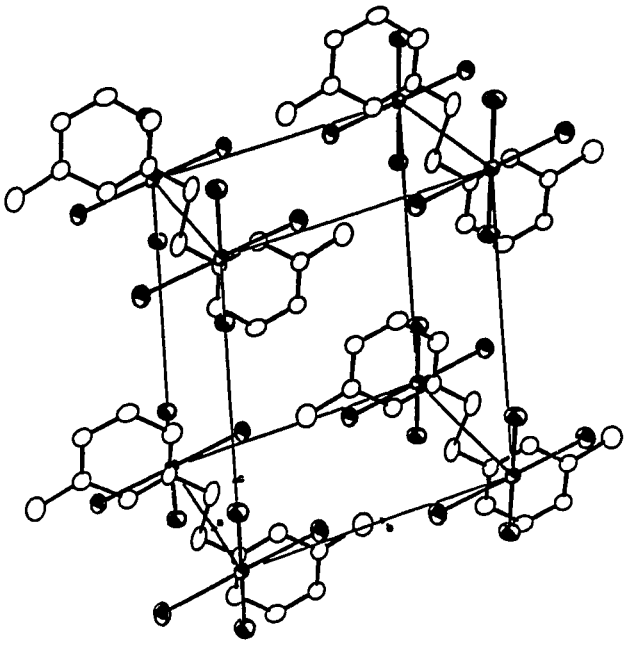
3.5.2: Structure of $[H(3\text{-picNO})_2]^+$ Cation in $[H(3\text{-picNO})_2][AuCl_4]$.

The atom-labelling scheme corresponding to Table VII, together with the distances and angles for $[H(3\text{-picNO})_2][AuCl_4]$ are given in Figure 10 and Table XII. The molecular packing showing relative orientation of $[H(3\text{-picNO})_2]^+$ cations and $[AuCl_4]^-$ anions in the unit cell is shown in Figure 11. The crystallographic asymmetric unit constitutes half a gold atom, two chlorine atoms and one 3-picNO molecule. The unit cell packing in this compound differs from that of the analogous diadduct of $[H(2\text{-picNO})_2][AuCl_4]$, but resembles that of other similar compounds of pyNO and it's derivatives such as $[H(pyNO)_2][AuCl_4]$, $[H(2\text{-picNO})_2]Cl.3H_2O$, $[H(2,6(CH_3)_2pyNO)_2][ClO_4]$ and $[H(dma)_2][AuCl_4]$, all of which have symmetry-restricted short hydrogen bond. The square

planar $[AuCl_4]^-$ units are stacked above one another but the distance between the adjacent metal atoms is quite large forbidding any metal-metal interactions, characteristic of super-conducting metallic compounds [69] such as $[Ni(dmg)_2]$, $[Pd(dmg)_2]$ (dmg = dimethyl glyoxime) etc. The two planar 3-picNO moieties in the dimeric cation $[H(3\text{-picNO})_2]^+$ are related by an inversion symmetry with a symmetry-restricted hydrogen bond. No atom in the 3-picNO is more than 0.014(10)Å out of the least-squares plane defined by all non-hydrogen atoms in the molecule. The unit cell packing allows enough open space for solvent molecules although no solvent of crystallization was present. There are no significant hydrogen bonding interactions between adjacent $[AuCl_4]^-$ and $[H(3\text{-picNO})_2]^+$ ions.

Table XII. Selected Bond Length (Å) and Angles (°) in $[H(3\text{-picNO})_2][AuCl_4]$.

(a) Bonding distances			
Au-Cl(1)	2.275(3)	Au-Cl(2)	2.286(3)
O(1)-N(2)	1.361(11)	N(2)-C(7)	1.340(14)
N(2)-C(3)	1.333(14)	C(3)-C(4)	1.405(13)
C(4)-C(5)	1.395(15)	C(5)-C(6)	1.381(16)
C(6)-C(7)	1.386(14)	C(4)-C(8)	1.502(16)
OHO-O(1)	1.080(0)		
(b) Bonding angles			
Cl(1)-Au-Cl(2)	89.8(1)	N(2)-O(1)-OHO	109.8(6)
O(1)-N(2)-C(3)	118.1(9)	O(1)-N(2)-C(7)	117.4(1.0)
N(2)-C(3)-C(4)	119.0(1.0)	N(2)-C(7)-C(6)	118.8(1.0)
C(3)-C(4)-C(5)	117.6(1.0)	C(3)-C(4)-C(8)	117.7(1.0)
C(3)-N(2)-C(7)	124.4(9)	C(4)-C(5)-C(6)	117.1(1.5)
C(4)-C(5)-C(8)	120.9(1.6)	C(5)-C(6)-C(7)	118.9(1.0)
C(5)-C(4)-C(8)	124.6(0.9)	C(6)-C(5)-C(8)	121.9(1.5)
(c) Non-bonding distances and angles			
Cl(1)---Cl(2)	3.231	Cl(1)---Au---Cl(1)	180.0
Cl(1)---Cl(2)	3.219	Cl(2)---Au---Cl(2)	180.00
O(1)---O(1)	2.406(9)		
Au---O(1)	3.039(3)		



Molecular packing depicting relative orientation of $[H(3\text{-picNO})_2][AuCl_4]$ in the triclinic unit cell, viewed along the 'a' axis.

Table XIII. Least-square Planes and Dihedral Angles of $[H(3\text{-picNO})_2][AuCl_4]$.

Plane 1 : $AuCl_4^-$ Anion

$-0.385X - 0.909Y - 0.159Z + 0.695 = 0$

Au	0.695(0)		
Cl(1)	1.078(4)	Cl(3)	-1.426(4)
Cl(2)	-0.935(4)	Cl(4)	0.588(4)

Plane 2 : 3-picNO (Molecule I)

$0.985X - 0.166Y - 0.041Z + 0.636 = 0$

O(1)	-0.011(10)	C(5)	-0.010(11)
N(2)	0.010(10)	C(6)	-0.003(11)
C(3)	-0.002(11)	C(7)	0.006(11)
C(4)	-0.014(11)	C(8)	-0.004(13)

Plane 3 : 3-picNO (Molecule II)

$0.985X - 0.167Y - 0.040Z - 0.449 = 0$

O(9)	0.010(10)	C(13)	0.013(11)
N(10)	-0.010(10)	C(14)	0.002(11)
C(11)	-0.005(11)	C(15)	-0.013(11)
C(12)	0.000(11)	C(16)	0.003(13)

Dihedral Angles

Plane 1	Plane 2	Angle (°)
1	2	102.8

The geometry of 3-picNO is normal with internal bond angles varying from 124.2 to 117.2°. The N-O bond length of 1.362(4)Å is not significantly different from the corresponding distance of 1.358(2)Å in the hydrogen-bonded diadduct, $[H(2\text{-picNO})_2]Cl.3H_2O$ [26] or 1.352(9)Å in $[Zn(4\text{-picNO})_6][ClO_4]_2$ [69] which has monodentate 4-picNO. The position of the electron-donating $-CH_3$ group on pyNO ring does not appear to make any significant difference on N-O bond or O---O separation. The average lengths for CH_3-C, C-C and C-N bonds and angles involving these bonds

are in agreement with the corresponding values in other similar compounds.

3.5.3: Structure of $[H(4\text{-picNO})_2]^+$ cation in $[H(4\text{-picNO})_2][AuCl_4]$.

The atom-labeling scheme and the packing of $[H(4\text{-picNO})_2]^+$ and $[AuCl_4]^-$ ions in the unit cell are shown in Figures 10 and 12, respectively. All relevant distances and angles are listed in Table XIV . The molecular packing in the present compound is essentially similar to $[AuCl_4]^-$-stabilized protonated diadducts of pyNO and 3-picNO which have symmetry-restricted short hydrogen bond.

Table XIV. Selected Bond Length (Å) and Angles (°) in $[H(4\text{-picNO})_2][AuCl_4]$.

(a) Bonding distances			
Au-Cl(1)	2.281(5)	C(4)-C(5)	1.37(3)
Au-Cl(2)	2.277(4)	C(8)-C(5)	1.51(3)
OHO-O(1)	1.517(2)	N(2)-C(7)	1.36(2)
OHO-O(1)	1.122(2)	C(6)-C(7)	1.36(3)
N(2)-O(1)	1.34(2)	C(5)-C(4)	1.37(3)
N(2)-C(3)	1.32(2)	C(5)-C(6)	1.39(2)
C(3)-N(2)	1.32(2)	C(5)-C(8)	1.51(3)
C(7)-N(2)	1.36(2)	C(4)-C(3)	1.37(3)
(b) Bonding angles			
C(5)-C(4)-C(3)	121.1(1.6)	C(6)-C(5)-C(4)	117.1(1.5)
C(4)-C(3)-N(2)	120.7(1.6)	C(8)-C(5)-C(4)	120.9(1.6)
C(7)-N(2)-O(1)	117.9(1.4)	C(8)-C(5)-C(6)	121.9(1.5)
C(7)-N(2)-C(3)	120.3(1.5)	C(7)-C(6)-C(5)	120.4(1.4)
C(3)-N(2)-O(1)	121.7(1.4)	C(6)-C(7)-N(2)	120.3(1.5)
Cl(2)-Au-Cl(1)	89.4(2)		
(c) Non-bonding distances and angles			
Cl(1)---Cl(2)	3.206(4)	Cl(1)---Au---Cl(1)[a]	179.96
Cl(1)---Cl(2)[a]	3.240(4)	Cl(2)---Au---Cl(2)[a]	180.00
O(1)---O(1)	2.442(4)		
Au---O(1)	3.200(5)		

a. On symmetry related positions.

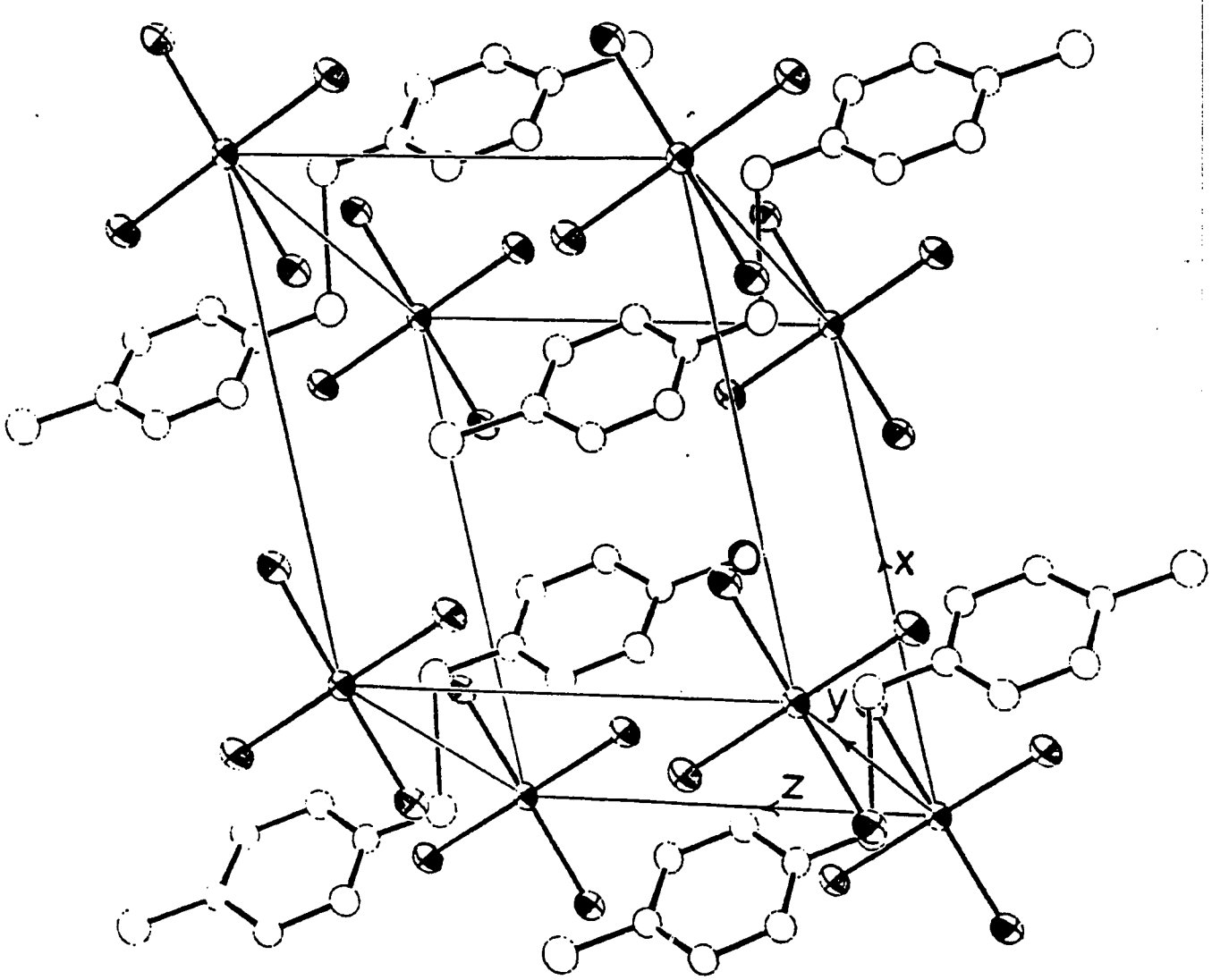


Figure 12: Molecular packing showing relative orientation of $[AuCl_4]^-$ and $[H(4\text{-picNO})_2]^+$ ions in the triclinic unit cell viewed along 'b' axis.

3.5.4: A Comparison of Crystallographic Studies of the Three Picoline N-oxide Compounds.

In $[H(4\text{-picNO})_2][AuCl_4]$ the internal bonds parallel to the molecular axis are slightly shorter than the other C-C bonds, as has been generally observed in aromatic compounds with para-substituents, indicating a contribution of quinoid resonance structures. The C-C bond length shortening to ℓ_{ave}= 1.365(1)Å is very small compared to ℓ_{ave}= 1.388(2)Å. The N=O bond length of 1.341(9)Å in the 4-picNO diadduct is not significantly different for 1.345(8)Å or 1.362(4)Å in the corresponding 2- and 3-picNO diadducts or 1.352(9)Å in $[Zn(4\text{-picNO})_6][ClO_4]$ which has a monodentate 4-picNO [69] (Table XV). Nevertheless, as indicated by the n.m.r. data, the $-CH_3$ substituents at 2- and 4- positions of the pyNO appear to have similar effects on the N=O bond length as compared to the $-CH_3$ at 3- position.

Table XV. Crystallographic Data for some Diadducts of Pyridine N-oxides .

Compound	symmetry	N - O	O---O	Ref.
$[NO_2\text{-pyNO}]$	Pnma	1.298(2)	-	71
[pyNO]	$P2_1$	1.35(2)	-	72
$[H(pyNO)_2][AuCl_4]$	$P\bar{1}$	1.362	2.41(1)	24
$[H(2\text{-picNO})_2][AuCl_4]$	$P2_1/n$	1.345(8)	2.393(6)	-
$[H(3\text{-picNO})_2][AuCl_4]$	$P\bar{1}$	1.359(4)	2.371(9)	-
$[H(4\text{-picNO})_2][AuCl_4]$	$P\bar{1}$	1.341(9)	2.442(9)	-

The similarity of N=O distance for gold(III) chloride compounds of 2- and 4-picNO and difference from that in 3-picNO compound, are expected from enhanced contribution of a similar set of resonance structures resulting from the electron-donating substituent ($-CH_3$) at the 2- and 4-positions [8].

3.5.5: Gold(III) Environment.

The $[AuCl_4]^-$ geometry is shown in Figure 13. In $[H(2\text{-picNO})_2][AuCl_4]$, the $[AuCl_4]^-$ ion is square-planar with the four Au-Cl distances rather variable. The average Au-Cl distance of 2.268(2)Å is equal to the value of 2.27(1)Å reported [46] as the most accurate value for the Au-Cl bond. The Au and four Cl atoms are coplanar (Plane 1:Table X) but the formal crystallographic symmetry of the ion is lower than the ideal 4/mm. The closest atoms to the Au other than Cl atoms, are O(1) atom at 3.240Å and N(2) atom at 3.712Å excluding any possibilities of coordination of these atoms to the gold. The distances involving hydrogen atoms are quite normal without any intermolecular hydrogen bonds.

In $[H(3\text{-picNO})_2][AuCl_4]$, the immediate metal environment may be considered square planar with chlorine atoms at an average distance of 2.280(3)Å and Cl(1)-Au-Cl(2) angle of 89.8(1)°. The oxygen atoms of N=O are at 3.039(3)Å from Au completing a distorted octahedron (Table XII and Figure 14) around the metal atom. Gold(III) will have an uncommon six-coordinate geometry if Au--O(1) interactions are considered real and not a manifestation of the packing forces in the unit cell. The Au--O contacts in this compound and other similar contacts of 3.105(7)Å and 3.240(3)Å in

$[H(pyNO)_2][AuCl_4]$ [24] and $[H(2\text{-}picNO)_2][AuCl_4]$ are close to 3.20Å, the sum of van der Waals radii [72] of the interacting atoms. Heterocyclic N-oxides have high dipole moments. A combination of dipole-dipole interactions and the above van der Waals interionic contacts should be the most dominant factors in packing of the crystal lattice in which gold(III) is in a distorted octahedral environment.

In $[H(4\text{-}picNO)_2][AuCl_4]$, the immediate environment of the metal is also approximately square planar with Au-Cl average distance of 2.279(5)Å and Cl(1)-Au-Cl(2) angle of 89.4(2)°. The O(1) atoms of two separate N-oxides moieties are at 3.202(5)Å on opposite sides of the planar $[AuCl_4]^-$ anion resulting in a distorted octahedral environment around the metal atom as shown in Figure 14. In this case, again a weak interaction, if any, of O(1) atoms with Au(III) depicts an unusual six-coordination for Au(III) which is a combined effect of factors such as mutual interactions of highly polar picNO (μ = 4.24 D) and unique packing arrangement of the molecules in the unit cell. Such six-coordinated Au(III) species are not expected to exist in solutions because of the lack of packing forces.

All dimeric cations can be structurally viewed analogous to the well-known $[H_5O_2]^+$ cation [64]. The aromatic N-oxide moiety in these cations is free to rotate about the O-H-O axis with the proton being equally shared by the oxygen atoms. The orientation of the two N-oxides moieties is essentially dictated by the packing forces in the unit cell.

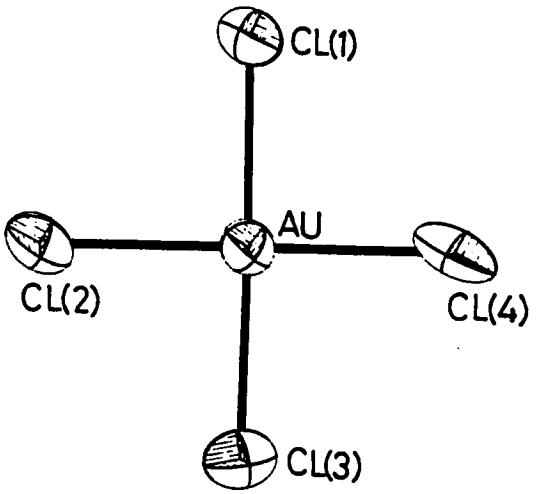


Figure 13: ORTEP diagram (50 % probability ellipsoids) showing relative thermal motion of atoms in the $[AuCl_4]^-$ anion in $[H(X\text{-}pyNO)_2][AuCl_4]$ where X = 2-Me, 3-Me or 4-Me.

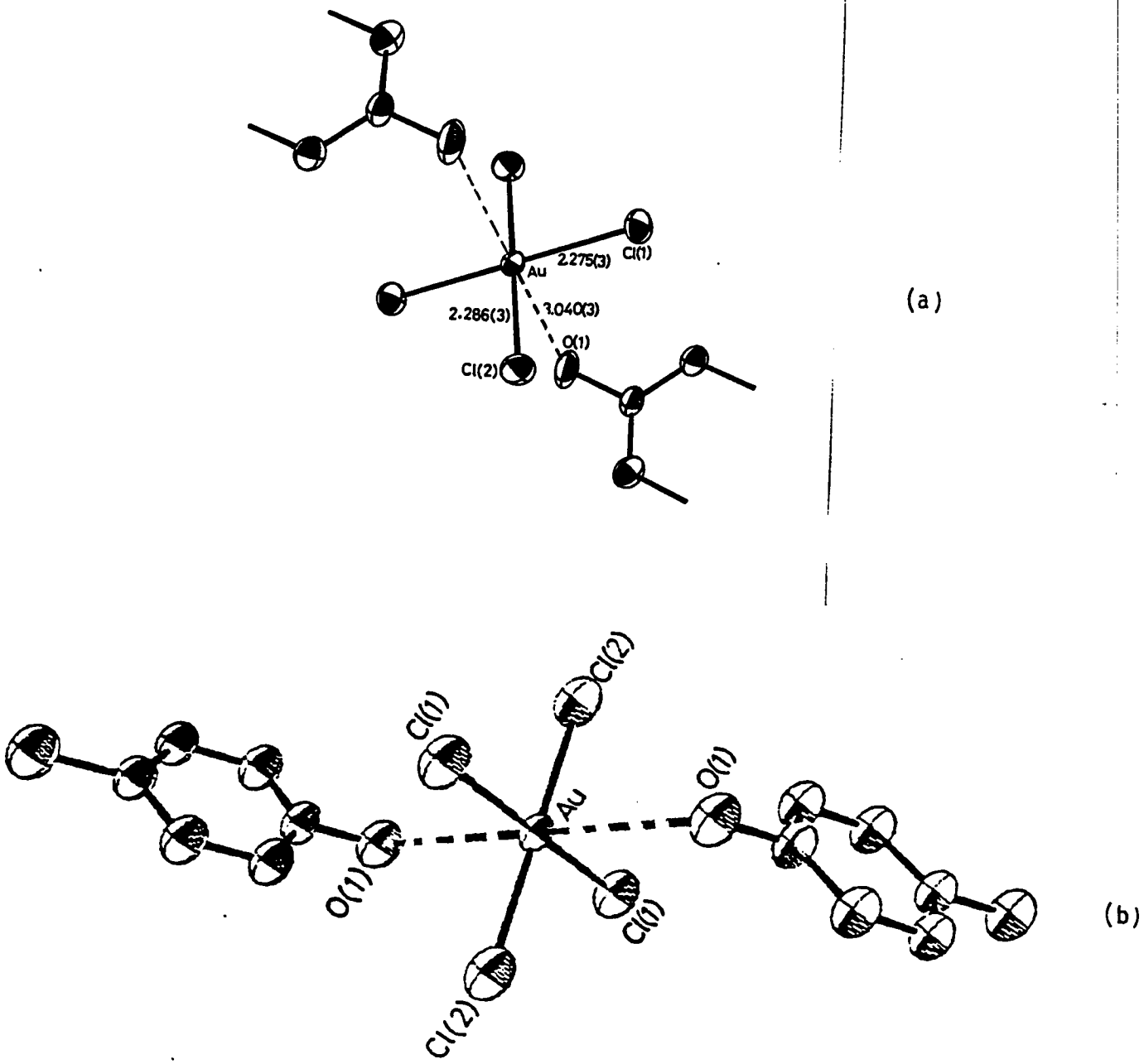


Figure 14: The environment of Gold(III) in the crystal lattices of: (a) $[H(3\text{-picNO})_2][AuCl_4]$ and (b) $[H(4\text{-picNO})_2][AuCl_4]$ depicting a distorted octahedral coordination around the metal atom.

3.5.6: The Short Hydrogen Bonding.

Despite the lack of symmetry constraints, the hydrogen bond in the dimeric cation $[H(2\text{-picNO})_2]^+$ is "very short" with O---O distance of 2.393(6)Å close to the mean value of 2.445(2)Å observed in Type A salts of monocarboxylic acids [20]. The most reasonable position of the proton obtained from the difference map is somewhat off-centre, its distances from O-atom are 1.416(11)Å and 1.148(10)Å. Such a difference fits the idea of a shallow potential energy well perhaps non-parabolic in shape for the short-hydrogen-bond and may be explained on the basis of environmental differences of the two oxygen atoms. There was no indication of a second hydrogen position near O(1) as might be expected for a double minimum potential of sufficient barrier height [35] and the occupancy of the OHO atom refined close to unity. However, conclusions about bridged hydrogen may be considered with caution because the x-ray analysis is unlikely to locate a H-atom accurately in the presence of heavy atom such as Au and Cl, even if the convergence during least-squares refinement was excellent (R = 3.90 %).

The inversion-symmetry related hydrogen bond in the dimeric cation, $[H(3\text{-picNO})_2]^+$ is 'very short' with O---O separation of 2.406(9)Å, close to the shortest O---O distance of 2.29(2)Å reported [9] in $[H_3O_2]^+$ ion which also has an inversion symmetry. The intramolecular hydrogen bonding distance is within the range of 2.310-2.626Å considered [64] for short hydrogen bond. The O---O separation of 2.442(9)Å in the 4-picNO diadduct is longer than the corresponding distances 2.393(6)Å in 2-picNO and the 2.406(9)Å in the 3-picNO diadducts (Table XIV). The bridging proton in

the dimeric cation is centered as required by the space group symmetry. Because of symmetry-restriction in the 3-picNO and 4-picNO dimeric cations a clear-cut distinction can not be made between a perfectly centered and a disordered hydrogen atom in the short hydrogen bond.

A chemical potential with either a single or a double-minimum would be appropriate to describe the energetics of the short hydrogen bond in $[H(3\text{-picNO})_2]^+$ and $[H(4\text{-picNO})_2]^+$ cations.

The electron density map and the overlap density fuctions are plotted in Figures 15 and 16 for the $[H(4\text{-picNO})_2][AuCl_4]$. The positive electron density is shown by lines whereas the density holes are drawn with dots. In 4-picNO molecule, an unshared pair of electron clearly appears on the oxygen of the N=O group while the other is involved in hydrogen bonding with an inversion symmetry on the hydrogen atom of the O-H-O bond. A hole in the electron density also clearly appears in the planar 4-picNO molecule, as expected for an aromatic ring system.

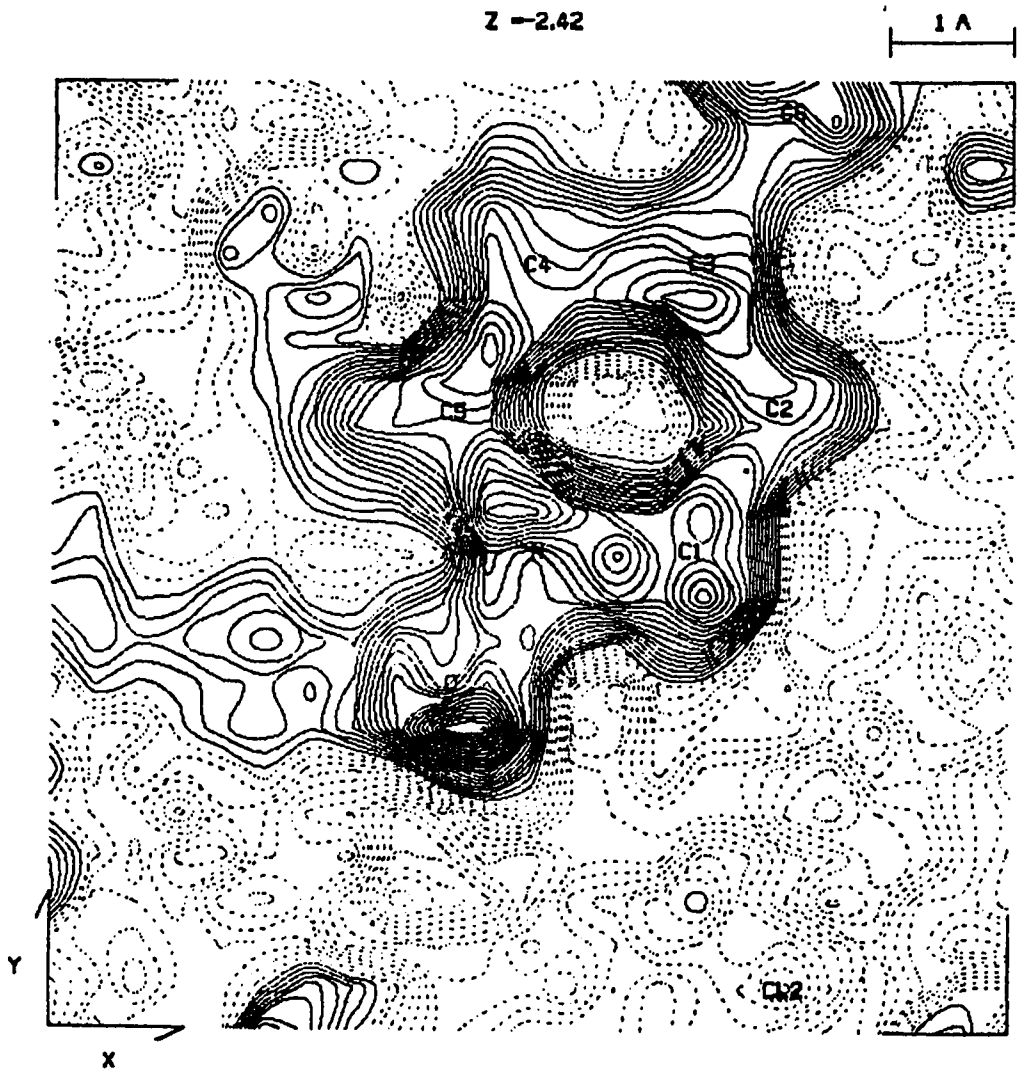


Figure 15: Electron density map for half of the $[H(4\text{-picNO})_2]^+$ cation showing unshared pair of electron on oxygen atom and the O-H bond.

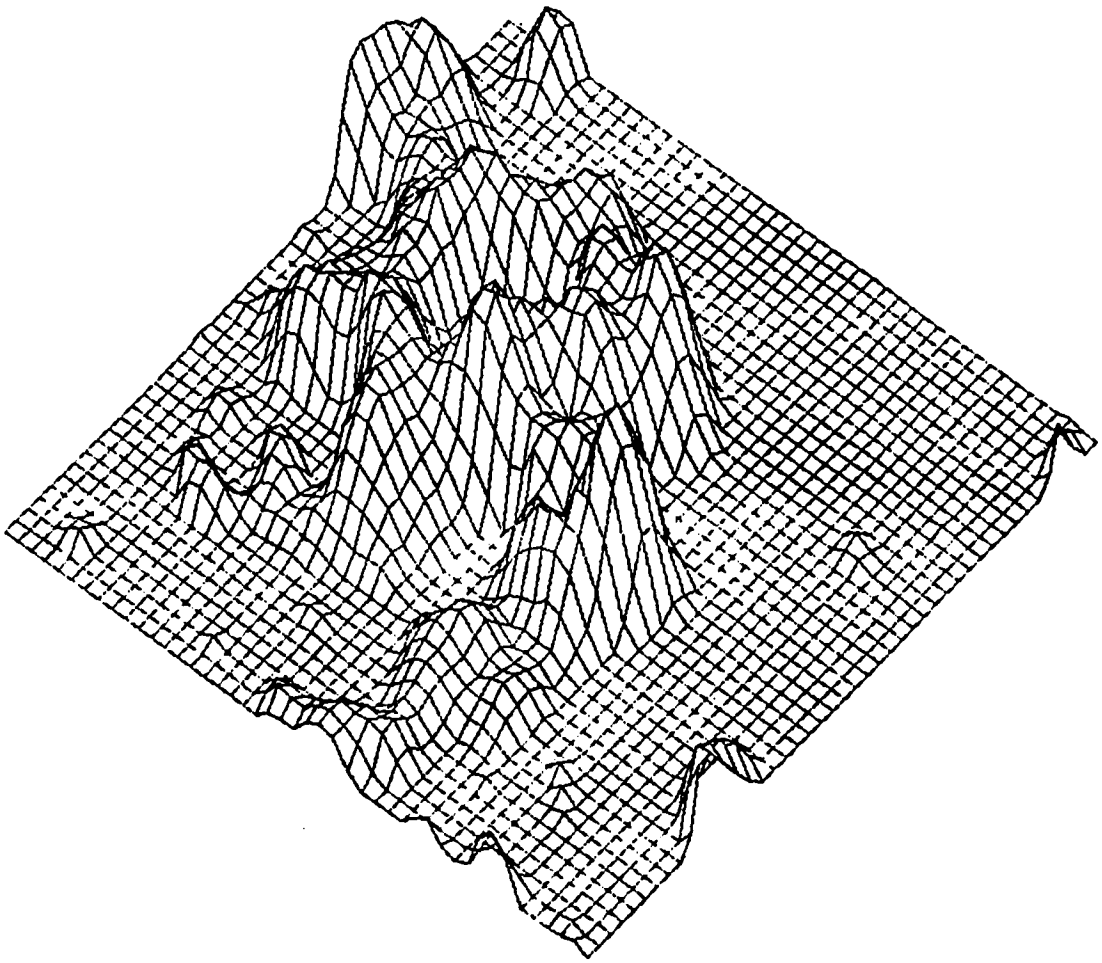


Figure 16: Overlap density function map (corresponding to Figure 15) for half of the $[H(4\text{-picNO})_2]^+$ cation.

CHAPTER FOUR

4. CONCLUSION

On the basis of the above investigations the following conclusions are drawn.

(1) In general, compounds of the formula $[H(R\text{-}pyNO)_2][AuCl_4]$ having short hydrogen-bonded dimeric cation, are formed.

(2) The O-H-O bond in the dimeric cations is among the shortest. In open symmetry-restricted O-H-O bond, the hydrogen atom is centered or disordered along O-H-O axis and a chemical potential with either a single or a double-minimum would be appropriate to describe the energetics of the bond.

(3) In the less common compounds with O-H-O bond without any symmetry-restrictions the chemical potentials for the hydrogen atom can be best described as a shallow potential energy well perhaps non-parabolic in shape.

(4) The existance of short hydrogen bond can be detected as a strong and broad absorption band around 1050 cm^{-1} in the i.r. spectra. In some compounds the resonance of the short hydrogen-bonded proton in the dimeric cations appears at about 10.0 p.p.m. in the proton n.m.r. spectra as compared to 18.0 p.p.m. for the intramolecular short hydrogen bond in chelated structures. However, spectroscopic data alone are not sufficient to describe the complete structures.

(5) Substituted heterocyclic N-oxides are potentially useful extractive-photometric reagents for extraction and determination of gold because of the high extinction coefficients of the products formed. However, further work is required in this area.

CHAPTER FIVE

5. REFERENCES

1. A.R. Katritzky, E.W. Randall and L.E. Sutton, J. Chem. Soc., 1769 (1957).

2. A.N. Sharpe and S. Walker, ibid., 4522 (1961).

3. E.P. Linton, J. Am. Chem. Soc., 62, 1945 (1940).

4. T. Kubota, ibid., 87, 458 (1965).

5. E. Ochiai, 'Aromatic Amine Oxides', American Elsevier Publishing company., (1967).

6. R.A. Barnes, J. Am. Chem. Soc., 81, 1935 (1959).

7. A.R. Katritzky and J.M. Lagowski, 'Chemistry of the Heterocyclic N-oxides', Academic Press, Chapter II, pp 160-165 (1971).

8. R.G. Garvey, J.H. Nelson and R.O. Ragsdale, Coordin. Chem. Rev., 3, 375 (1968).

9. J.V. Quagliano, J. Fujita, G. Franz, D.J. Phillips, J.A. Walmsley and S.Y. Tyrel, J. Am. Chem. Soc., 83, 3770 (1961).

10. C.P. Keijzers, G. Van Kalkern, E. de Boer and J.S. Wood, Mol. Phys., 49, 1187 (1983).

11. J.S. Wood, R.O. Day, C.P. Keijzers, E. de Boer, A.E. Yildirim and A.A.K. Klaasen, Inorg. Chem., 20, 1982 (1981).

12. M. Orchin and P.J. Schmidt, Coordin. Chem. Rev., 3, 345 (1968).

13. L. Garcia and M. Orchin, J. Chem. Soc., 2254 (1961).

14. W.E. Hatfield, Y. Muto, H.B. Jonassen and J.S. Paschal, Inorg. chem., 4, 97 (1965).

15. P. Knuuttila, Polyhedron, 3, 303 (1984).

16. H. Freiser, Q. Fernando and P.J. Sun., Anal. Chem., 36, 2485 (1964).

17. H. Yoneda, G.R. Choppin, J.L. Bear and A.J. Graffeo, Inorg. Chem., 4, 244 (1965).

18. H. Sigel and H. Brintzinger, Helv. Chim. Acta, 26, 701 (1963).

19. J.O. Lundgren and I. Olovsson, 'The Hydrogen Bond', ed., P. Schuster G. Zundel and C. Sandorfy, North-Holland, Amesterdam, Ch. 10, pp 473-526 (1976).

20. J.C. Speakman, "Structure and Bonding", 12, 141 (1972).

21. M. S. Hussain and E.O. Schlemper, J. Chem. Soc., Dalton Trans., 750-755 (1980).

22. A.G. Galinos, J. Am. Chem. Soc., 82, 3032 (1960).

23. P.G. Jones and G.M. Sheldrick, Acta Crystallogr., B34, 1353 (1978).

24. M. S. Hussain and E.O. Schlemper, J. Chem. Soc., Dalton Trans., 751 (1982)

25. H.H. Mills and J.C. Speakman, Proc. Chem. Soc., 216 (1963).

26. J.C. Speakman and K.W. Muir, Croat. Chem. Acta., 55, 233 (1982).

27. M. Jaskolki, M. Gdaniec, Z. Kosturkiewicz and M. Szafran, Pol. J. Chem., 52, 2399 (1978).

28. A.G. Galinos, J. Inorg. Nucl. Chem., 19, 69 (1961).

29. B.E.V. Salinas and E.O. Schlemper, J. Cryst. Mol. Struct, 8, 217 (1978).

30. R. Clements and J.L. Wood, J. Cryst. Mol. Struct., 17, 265 (1973)

31. R. Clements and J.L. Wood, ibid, 17, 291 (1973).

32. M. Ziegler, P.B.Barth, and H. Winkler, Angew. Chem. Internal. Edn., 8, 980 (1969).

33. M. Ziegler and G. Stephan, Mickrochim Acta., 628 (1970).

34. M. Ziegler and H. Winkler, Mickrochim Acta., 457 (1976).

35. G.S. Harris F. Inglis, J. Mckechnic, K.K. Cheung and G. Ferguson, J.C.S. Chem. Comm., 442 (1967).

36. W. Conschorek and H. Kuppers, Acta Cryst., B31, 1068 (1975).

37. M. S. Hussain, E.O. Schlemper and C.K. Fair, Acta Cryst., B36, 1104 (1980) and references therein.

38. M. S. Hussain, E.O. Schlemper and W.B. Yelon, Acta Crystallogr., B37, 437 (1981) .

39. M. S. Hussain and E.O. Schlemper, Inorg. Chem., 18, 1116-1121 (1979).

40. M. S. Hussain and E.O. Schlemper, Inorg. Chem., 18, 2275-2282

(1979).

41. M. S. Hussain, B. Salinas and E.O. Schlemper, Acta Cryst., B35, 628-633 (1979).

42. M. S. Hussain, Arabian J. Sci. Engineering, 8, 355-367 (1983); and references therein.

43. J. Kroon, J.A. Kanters and A.F. Peerdeman, Nature (London), 229, 120 (1971).

44. M. Catti and G. Ferraris, Acta Cryst., B32, 2754 (1976).

45. D.H. Brown and W.E. Smith, Chem. Soc. Rev., 9, 217 (1980).

46. P.G. Jones., Gold Bull., 14, 102 (1981).

47. C. F. Shaw, Inorg. Perspect. Biol. Med., 2, 278 (1979).

48. R. W. Mason, Pharmacology, 15, 536 (1977).

49. D. T. Walz, M. J. Dimartino and B. M. Sutton, "Anti-Inflammatory Agents', Academic Press, New York, 1974, Vol.1, p 217.

50. S. L. Lawton, TRACERII-Lattice Transformation-Cell Reduction computer program (Northwestern Version), April 1967.

51. MULTAN82, A Recent Version of Crystallographic Program Package of. P. Main et. al., University of York, York, England.

52. G.M. Sheldrick, SHELX76 Program for Crystal Structure Determination, University of Cambridge, England.

53. D.T. Cromer and J.B. Mann, Acta Crystallogr., A24, 321 (1968).

54. R. F. Stewart, E. R. Davidson and W. T. Simpson, J. Chem. Phys., 42, 3175 (1965)

55. D.T. Cromer and D. Liberman, J. Chem. Phys., 53, 1891 (1970).

56. Molecular Structure Corporation, Stand-Alone Structure Determination Package including PDP11/23, Array Processor, Magnetic Tape Drive, Diskette Drive, Prism 132 Printer , VT-100/CIT-414 terminal combination and SDP82 software.

57. D. H. Brown and W. E. Smith, J. Chem. Soc., Dalton Trans., 848 (1976).

58. M.F. Clayer and N. Sheppard, Chem. Commun., 1431 (1969).

59. D. Hadzi, Pure Appl. Chem., 11, 435 (1965).

60. D. Hadzi, J. Chem. Soc., 5128 (1962).

61. B. P. Mishra and D. V. R. Rao, J. Indian. Chem. Soc., LVI, 238 (1979).

62. J.S. Martin and F.Y. Fujiwara, Cand. J. Chem., 49, 3071 (1971).

63. R.M. Silverstein, G.C. Bassler and T.C. Marrill, "Spectroscopic Identification of Organic Compounds", John Wiley and Sons, Inc. p 197, (1981).

64. J. Emsley, Chem. Soc. Rev., 91 (1980).

65. P.G. Jones and G.M. Sheldrick, Acta Crystallogr., B34, 1353 (1978).

66. R.A. Penneman and R.R. Ryan, Acta Crystallogr., B28, 1629 (1972).

67. J.M. Williams and S.W. Peterson, J. Am. Chem. Soc., 91, 776-777 (1969).

68. W. Conschorek and H. Kuppers, Acta Cryst., B31, 1068 (1975).

69. A. E. Underhill and D. M. Watkins, Chem. Soc. Rev., 9, 429 (1980).

70. J. S. Wood, R. O. Day, C. P. Keijzers, E. de Boer, A. E. Yildirim and A. A. K. Klaasen, Inorg. Chem., 20, 1981 (1982).

71. Wang, Y., Blessing, R.H., Ross, F.K. and Coppens, P., Acta cryst., B32, 52 (1976)

72. Ulku, D., Huddle, B.P. and Morrow, J.C., Acta Cryst., B27, 432 (1971).

73. A. Bondi, J. Phys. Chem., 68, 441 (1964).

APPENDIX A

Structure Factor Tables for $[H(2\text{-picNO})_2][AuCl_4]$, $[H(3\text{-picNO})_2][AuCl_4]$ and $[H(4\text{-picNO})_2][AuCl_4]$

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(2-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	0	0	455	-397	10	2	0	877	-867	8	4	0	99	43	14	6	0	409	-405	12	9	0	257	-259
4	0	0	3133	-3902	11	2	0	1407	1435	9	4	0	1327	-1340	15	6	0	863	-842	13	9	0	289	286
6	0	0	113	-60	12	2	0	1204	1209	10	4	0	761	749	16	6	0	747	750	14	9	0	530	523
8	0	0	492	494	13	2	0	397	-405	11	4	0	1320	-1346	17	6	0	137	116	15	9	0	212	-191
10	0	0	403	397	14	2	0	349	331	13	4	0	577	587	18	6	0	216	213	16	9	0	248	229
12	0	0	1871	-1870	15	2	0	914	-904	14	4	0	295	-295	19	6	0	635	649	0	10	0	668	665
14	0	0	965	-925	16	2	0	899	-870	15	4	0	695	698	20	6	0	459	-460	1	10	0	399	-402
16	0	0	1820	1745	17	2	0	123	111	17	4	0	298	-283	22	6	0	160	-200	3	10	0	560	-564
18	0	0	529	516	18	2	0	301	-306	18	4	0	245	-255	1	7	0	548	-535	4	10	0	516	-522
20	0	0	617	-606	19	2	0	635	625	19	4	0	986	-996	2	7	0	1487	1505	5	10	0	226	201
22	0	0	279	-284	20	2	0	517	513	21	4	0	129	137	3	7	0	243	-232	6	10	0	135	-32
24	0	0	369	373	21	2	0	286	-273	23	4	0	732	734	4	7	0	123	-103	7	10	0	439	415
26	0	0	441	396	22	2	0	501	498	1	5	0	1131	1140	5	7	0	693	694	8	10	0	392	376
1	1	0	569	540	23	2	0	652	-663	2	5	0	546	-538	6	7	0	1284	-1298	9	10	0	325	-351
2	1	0	1886	2486	24	2	0	413	-397	3	5	0	957	-966	7	7	0	226	-196	10	10	0	321	306
3	1	0	668	-668	26	2	0	231	-284	4	5	0	323	-330	8	7	0	226	-208	11	10	0	333	-338
4	1	0	534	540	1	3	0	673	-702	5	5	0	1407	-1423	9	7	0	122	-98	12	10	0	422	-394
5	1	0	348	-336	2	3	0	409	-408	6	5	0	680	692	10	7	0	1088	1056	13	10	0	334	319
6	1	0	1363	-1385	3	3	0	834	832	7	5	0	870	852	11	7	0	573	564	1	11	0	546	558
7	1	0	694	661	4	3	0	878	876	8	5	0	212	208	12	7	0	326	314	2	11	0	273	266
8	1	0	95	-61	5	3	0	2154	2327	9	5	0	1015	1000	13	7	0	149	164	3	11	0	451	-435
9	1	0	936	944	6	3	0	1052	1061	10	5	0	429	-417	14	7	0	827	-811	4	11	0	146	-115
10	1	0	1646	1651	7	3	0	1530	-1601	11	5	0	490	-494	16	7	0	247	-267	5	11	0	416	-416
11	1	0	569	-572	8	3	0	423	443	12	5	0	137	-125	17	7	0	331	-323	6	11	0	164	-144
12	1	0	444	439	9	3	0	2168	-2309	13	5	0	936	-933	18	7	0	609	596	7	11	0	273	276
13	1	0	1088	-1063	10	3	0	714	-717	14	5	0	518	514	20	7	0	206	227	8	11	0	186	-96
14	1	0	2002	-1985	11	3	0	928	975	15	5	0	527	552	21	7	0	241	242	9	11	0	329	336
16	1	0	618	-596	12	3	0	330	-346	16	5	0	227	259	0	8	0	1117	-1155	-25	0	1	192	208
17	1	0	545	551	13	3	0	979	998	17	5	0	1073	1112	3	8	0	234	-223	-23	0	1	834	-816
18	1	0	1073	1033	14	3	0	314	329	18	5	0	477	-493	4	8	0	1117	1096	-21	0	1	120	-161
19	1	0	259	-299	15	3	0	207	-195	19	5	0	358	-344	5	8	0	253	-239	-19	0	1	957	934
20	1	0	570	553	17	3	0	812	-810	20	5	0	314	-340	8	8	0	1073	-1061	-17	0	1	542	506
21	1	0	139	-189	18	3	0	541	-531	21	5	0	783	-804	10	8	0	353	-313	-15	0	1	1574	-1570
22	1	0	624	-590	19	3	0	314	324	22	5	0	301	290	11	8	0	181	158	-13	0	1	1458	-1464
23	1	0	234	226	20	3	0	121	-129	0	6	0	1711	1779	12	8	0	965	959	-11	0	1	1842	1873
24	1	0	344	-378	21	3	0	841	808	1	6	0	965	956	14	8	0	358	355	-9	0	1	1436	1485
25	1	0	252	322	22	3	0	297	309	2	6	0	387	-391	16	8	0	556	-551	-7	0	1	994	-1001
26	1	0	480	469	23	3	0	219	-220	3	6	0	1204	1227	17	8	0	202	209	-5	0	1	1204	-1211
0	2	0	1603	-1819	24	3	0	188	242	4	6	0	1392	-1408	18	8	0	169	-228	-3	0	1	1886	1923
1	2	0	812	799	25	3	0	597	-589	5	6	0	401	-359	1	9	0	373	-375	-1	0	1	1733	1971
2	2	0	210	197	0	4	0	351	-345	6	6	0	120	135	2	9	0	740	-732	1	0	1	1661	-2060
3	2	0	1523	1597	1	4	0	979	-940	7	6	0	870	-847	4	9	0	117	-71	3	0	1	2190	-2655
4	2	0	1610	1694	2	4	0	680	-658	8	6	0	827	801	5	9	0	480	484	5	0	1	1066	1077
5	2	0	1356	-1408	3	4	0	1711	-1758	9	6	0	534	528	6	9	0	769	781	7	0	1	635	647
6	2	0	555	545	4	4	0	237	-207	10	6	0	484	484	8	9	0	168	160	9	0	1	174	-163
7	2	0	1334	-1389	5	4	0	1639	1677	11	6	0	632	608	9	9	0	395	-377	11	0	1	1849	-1843
8	2	0	1458	-1527	6	4	0	576	531	12	6	0	651	-628	10	9	0	798	-784	13	0	1	599	583
9	2	0	1139	1122	7	4	0	2357	2452	13	6	0	422	-413	11	9	0	217	186	15	0	1	2328	2299

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(2-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
17	0	1	358	-355	22	1	1	290	281	22	2	1	278	-306	21	3	1	342	347	-20	5	1	337	345
19	0	1	1073	-1025	25	1	1	540	526	23	2	1	482	-511	22	3	1	776	-766	-18	5	1	1073	1108
21	0	1	119	115	26	1	1	182	-168	24	2	1	405	379	24	3	1	494	-489	-17	5	1	468	-487
23	0	1	530	525	-26	2	1	299	299	-25	3	1	226	-252	-24	4	1	493	-484	-16	5	1	583	-583
-25	1	1	680	686	-24	2	1	540	532	-24	3	1	268	292	-23	4	1	146	37	-15	5	1	301	-288
-22	1	1	374	-378	-23	2	1	640	636	-22	3	1	899	883	-22	4	1	304	290	-14	5	1	994	-1026
-21	1	1	722	-742	-21	2	1	178	-151	-21	3	1	389	387	-21	4	1	131	-176	-13	5	1	123	104
-19	1	1	421	-424	-20	2	1	769	-771	-20	3	1	332	-331	-20	4	1	1001	1019	-12	5	1	347	330
-18	1	1	330	336	-19	2	1	637	-634	-19	3	1	130	28	-18	4	1	323	-335	-11	5	1	345	335
-17	1	1	1044	1020	-18	2	1	259	254	-18	3	1	986	-992	-17	4	1	131	162	-10	5	1	994	965
-16	1	1	465	-464	-17	2	1	337	-316	-17	3	1	310	-308	-16	4	1	1189	-1244	-9	5	1	416	-400
-15	1	1	986	988	-16	2	1	725	716	-16	3	1	324	325	-14	4	1	270	270	-7	5	1	455	-447
-14	1	1	592	-628	-15	2	1	482	474	-15	3	1	350	-362	-13	4	1	203	209	-6	5	1	1799	-1812
-13	1	1	1537	-1539	-14	2	1	790	-798	-14	3	1	1175	1177	-12	4	1	1102	1098	-5	5	1	972	985
-12	1	1	899	922	-13	2	1	1131	1102	-13	3	1	416	434	-11	4	1	159	156	-4	5	1	304	-310
-11	1	1	1276	-1268	-12	2	1	1204	-1219	-12	3	1	372	-368	-10	4	1	322	-305	-3	5	1	877	847
-10	1	1	622	628	-11	2	1	1378	-1362	-11	3	1	107	75	-9	4	1	326	-309	-2	5	1	2038	2164
-9	1	1	1682	1718	-10	2	1	91	-62	-10	3	1	1849	-1988	-8	4	1	2060	-2091	-1	5	1	747	-711
-8	1	1	413	407	-9	2	1	957	-966	-9	3	1	686	-695	-7	4	1	148	97	0	5	1	193	185
-7	1	1	717	732	-8	2	1	1682	1767	-8	3	1	104	57	-6	4	1	307	297	1	5	1	653	-621
-6	1	1	480	-443	-7	2	1	2031	2215	-7	3	1	557	-517	-5	4	1	107	-77	2	5	1	1487	-1505
-5	1	1	1407	-1484	-6	2	1	624	619	-6	3	1	2473	2739	-4	4	1	2306	2545	3	5	1	207	199
-4	1	1	569	-552	-5	2	1	957	999	-5	3	1	390	370	-3	4	1	414	-403	4	5	1	321	-306
-3	1	1	1784	-1918	-4	2	1	1269	-1281	-4	3	1	222	-233	-2	4	1	175	169	5	5	1	551	525
-2	1	1	1095	1085	-3	2	1	965	-940	-3	3	1	1110	1105	-1	4	1	291	265	6	5	1	1508	1487
-1	1	1	2183	2493	-2	2	1	178	142	-2	3	1	1610	-1630	0	4	1	1668	-1732	7	5	1	319	-300
0	1	1	512	444	-1	2	1	1828	-1894	-1	3	1	273	241	1	4	1	711	-700	8	5	1	694	672
1	1	1	2161	2642	0	2	1	2219	2541	0	3	1	137	-139	2	4	1	139	-120	9	5	1	769	-780
2	1	1	1436	-1504	1	2	1	332	314	1	3	1	664	-636	3	4	1	761	718	10	5	1	1356	-1369
3	1	1	1574	-1712	2	2	1	461	-453	2	3	1	1436	1488	4	4	1	2052	2126	11	5	1	418	414
4	1	1	877	-854	3	2	1	2089	2290	3	3	1	856	800	5	4	1	461	470	12	5	1	435	-427
5	1	1	1342	-1398	4	2	1	2089	-2247	4	3	1	892	850	6	4	1	408	438	13	5	1	534	544
6	1	1	539	538	5	2	1	1421	-1452	5	3	1	776	754	7	4	1	335	-320	14	5	1	812	801
7	1	1	445	465	6	2	1	877	-877	6	3	1	2458	-2640	8	4	1	2161	-2264	15	5	1	183	-194
8	1	1	313	323	7	2	1	1487	-1558	7	3	1	740	-773	9	4	1	323	335	16	5	1	367	358
9	1	1	1487	1485	8	2	1	1661	1779	8	3	1	602	-609	10	4	1	637	-637	17	5	1	371	-369
10	1	1	356	-352	9	2	1	921	930	9	3	1	1102	-1084	12	4	1	1088	1105	18	5	1	666	-653
11	1	1	747	-762	10	2	1	490	475	10	3	1	1806	1884	13	4	1	363	-361	20	5	1	383	-388
12	1	1	271	-281	11	2	1	1001	1003	11	3	1	275	-265	14	4	1	533	554	21	5	1	191	208
13	1	1	1893	-1884	12	2	1	1052	-1061	12	3	1	260	276	15	4	1	130	70	22	5	1	458	468
14	1	1	705	684	13	2	1	231	-234	13	3	1	611	608	16	4	1	725	-742	-22	6	1	139	-157
15	1	1	518	508	14	2	1	407	-438	14	3	1	805	-816	17	4	1	141	-176	-21	6	1	110	-115
16	1	1	202	234	15	2	1	761	-780	15	3	1	173	-160	18	4	1	632	-627	-20	6	1	470	-485
17	1	1	1392	1339	16	2	1	682	691	16	3	1	433	-432	20	4	1	790	787	-19	6	1	601	629
18	1	1	376	-372	17	2	1	213	234	17	3	1	146	-217	22	4	1	623	624	-18	6	1	359	370
19	1	1	174	-141	18	2	1	373	388	18	3	1	680	692	24	4	1	516	-486	-17	6	1	450	441
20	1	1	193	-186	19	2	1	673	712	19	3	1	260	304	-22	5	1	506	-514	-16	6	1	680	669
21	1	1	558	-551	20	2	1	522	-531	20	3	1	769	772	-21	5	1	362	368	-15	6	1	624	-616

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(2-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-14	6	1	331	-311	-10	7	1	427	-416	4	8	1	178	-140	-5	10	1	355	-311	20	0	2	557	534
-13	6	1	607	-585	-9	7	1	841	826	5	8	1	601	-589	-4	10	1	540	530	22	0	2	405	403
-12	6	1	566	-535	-8	7	1	233	-208	7	8	1	921	-926	-3	10	1	177	133	24	0	2	334	-319
-11	6	1	600	585	-7	7	1	656	656	9	8	1	421	403	-1	10	1	429	464	-26	1	2	497	480
-10	6	1	125	-112	-6	7	1	416	414	10	8	1	223	219	0	10	1	661	-658	-25	1	2	220	-253
-9	6	1	464	459	-5	7	1	732	-712	11	8	1	725	713	1	10	1	407	-429	-24	1	2	374	-356
-8	6	1	747	723	-4	7	1	447	-446	12	8	1	142	50	2	10	1	198	-211	-23	1	2	315	-319
-7	6	1	877	-869	-3	7	1	957	-970	13	8	1	228	-210	3	10	1	426	-436	-22	1	2	783	-761
-6	6	1	105	16	-2	7	1	463	-477	15	8	1	666	-670	4	10	1	585	589	-20	1	2	520	512
-5	6	1	986	-988	-1	7	1	863	850	16	8	1	119	123	5	10	1	494	475	-19	1	2	471	479
-4	6	1	1421	-1453	1	7	1	914	913	17	8	1	155	117	6	10	1	158	139	-18	1	2	878	884
-3	6	1	928	895	2	7	1	366	366	18	8	1	143	-116	7	10	1	360	357	-17	1	2	429	-432
-2	6	1	277	251	3	7	1	848	-819	19	8	1	540	539	8	10	1	405	-406	-15	1	2	99	116
-1	6	1	1160	1128	4	7	1	658	647	-17	9	1	323	-330	10	10	1	159	-36	-14	1	2	1443	-1495
0	6	1	1211	1236	5	7	1	870	-847	-15	9	1	208	-200	11	10	1	390	-387	-13	1	2	798	834
1	6	1	732	-703	6	7	1	401	-368	-14	9	1	342	366	12	10	1	400	404	-11	1	2	534	499
2	6	1	448	430	7	7	1	426	413	-13	9	1	667	661	-9	11	1	186	188	-10	1	2	1900	1961
3	6	1	670	-648	8	7	1	134	-127	-11	9	1	429	425	-6	11	1	500	-510	-9	1	2	203	-203
4	6	1	732	-715	9	7	1	1081	1082	-10	9	1	492	-472	-3	11	1	288	-279	-8	1	2	790	-736
5	6	1	725	727	10	7	1	642	644	-9	9	1	715	-716	-2	11	1	677	684	-7	1	2	1559	-1492
6	6	1	511	-505	11	7	1	152	-154	-8	9	1	133	105	-1	11	1	154	97	-6	1	2	1893	-1853
7	6	1	681	669	12	7	1	229	-207	-7	9	1	578	-575	0	11	1	149	82	-5	1	2	486	-454
8	6	1	732	717	13	7	1	1052	-1031	-6	9	1	243	232	1	11	1	143	205	-4	1	2	258	241
9	6	1	336	-336	14	7	1	373	-373	-5	9	1	400	428	2	11	1	651	-636	-3	1	2	1146	1138
10	6	1	241	231	15	7	1	265	253	-3	9	1	597	608	3	11	1	228	-217	-2	1	2	2234	2454
11	6	1	950	-956	16	7	1	262	-259	-2	9	1	266	-254	4	11	1	156	-154	-1	1	2	2002	-2198
12	6	1	957	-961	17	7	1	637	650	-1	9	1	463	-473	6	11	1	434	434	0	1	2	1849	1981
13	6	1	193	172	19	7	1	223	-168	0	9	1	128	-170	-26	0	2	305	-289	1	1	2	511	-464
14	6	1	297	-266	20	7	1	247	239	1	9	1	769	-802	-24	0	2	725	-719	2	1	2	2915	-3688
15	6	1	776	794	-19	8	1	373	-377	2	9	1	533	529	-22	0	2	371	380	3	1	2	2197	2432
16	6	1	624	611	-17	8	1	157	-189	3	9	1	593	578	-20	0	2	1255	1252	4	1	2	1545	-1607
17	6	1	258	-244	-15	8	1	541	527	4	9	1	219	192	-18	0	2	281	-257	5	1	2	700	726
18	6	1	395	393	-14	8	1	129	-29	5	9	1	827	839	-16	0	2	1501	-1510	6	1	2	2168	2338
19	6	1	532	-547	-13	8	1	605	580	6	9	1	544	-547	-14	0	2	173	173	7	1	2	85	36
20	6	1	245	-258	-11	8	1	979	-964	7	9	1	381	-387	-12	0	2	1886	1959	8	1	2	339	327
21	6	1	120	107	-10	8	1	183	174	9	9	1	679	-657	-8	0	2	2248	-2304	9	1	2	682	-702
22	6	1	241	-252	-9	8	1	870	-861	10	9	1	376	370	-6	0	2	185	173	10	1	2	1110	-1140
-21	7	1	413	-420	-8	8	1	190	-121	11	9	1	228	224	-4	0	2	2089	2088	11	1	2	106	-106
-20	7	1	168	-143	-7	8	1	1044	1022	12	9	1	146	-50	-2	0	2	477	463	12	1	2	754	-758
-19	7	1	282	-270	-6	8	1	126	130	13	9	1	567	548	2	0	2	776	-772	13	1	2	528	530
-18	7	1	213	-219	-5	8	1	610	632	14	9	1	261	-227	4	0	2	1175	1215	14	1	2	1146	1158
-17	7	1	686	671	-4	8	1	112	11	-13	10	1	131	-150	6	0	2	950	977	15	1	2	187	-203
-16	7	1	220	226	-3	8	1	776	-774	-12	10	1	506	513	8	0	2	1342	-1362	16	1	2	921	894
-15	7	1	502	500	-2	8	1	378	-391	-11	10	1	429	443	10	0	2	345	-355	17	1	2	480	-483
-14	7	1	305	276	-1	8	1	776	-774	-9	10	1	210	172	12	0	2	1878	1896	18	1	2	747	-721
-13	7	1	972	-966	0	8	1	164	159	-8	10	1	529	-532	14	0	2	885	859	20	1	2	554	-546
-12	7	1	140	193	1	8	1	740	733	-7	10	1	291	-276	16	0	2	1530	-1493	21	1	2	192	213
-11	7	1	489	-489	3	8	1	1052	1058	-6	10	1	136	98	18	0	2	834	-831	22	1	2	424	407

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(2-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
23	1	2	166	123	23	2	2	539	522	-24	4	2	171	-62	-14	5	2	584	561	-7	6	2	500	-480
24	1	2	316	313	24	2	2	300	307	-23	4	2	512	530	-13	5	2	856	814	-5	6	2	870	-892
-25	2	2	181	210	-25	3	2	593	591	-21	4	2	369	371	-12	5	2	297	297	-4	6	2	1313	1360
-24	2	2	479	490	-24	3	2	152	43	-19	4	2	979	-980	-11	5	2	353	323	-3	6	2	1146	1151
-23	2	2	501	-510	-23	3	2	262	275	-18	4	2	162	-161	-10	5	2	327	-336	-2	6	2	480	479
-22	2	2	321	-347	-22	3	2	192	222	-17	4	2	673	-680	-9	5	2	446	-434	-1	6	2	1001	999
-21	2	2	518	-516	-21	3	2	693	-703	-15	4	2	1153	1183	-8	5	2	313	314	0	6	2	1182	-1195
-20	2	2	590	-588	-20	3	2	217	-220	-14	4	2	293	297	-7	5	2	1081	-1107	1	6	2	892	-880
-19	2	2	347	342	-19	3	2	416	-412	-13	4	2	776	814	-6	5	2	834	829	2	6	2	303	-288
-18	2	2	181	169	-18	3	2	167	-186	-11	4	2	1015	-979	-5	5	2	1233	1243	3	6	2	669	-656
-17	2	2	264	268	-17	3	2	979	972	-10	4	2	126	128	-4	5	2	160	-149	4	6	2	740	716
-16	2	2	936	926	-15	3	2	429	421	-9	4	2	994	-988	-3	5	2	2002	2085	6	6	2	224	222
-15	2	2	914	-922	-14	3	2	499	471	-7	4	2	1182	1189	-2	5	2	965	-928	7	6	2	699	688
-14	2	2	461	471	-13	3	2	1146	-1138	-6	4	2	732	-699	-1	5	2	1487	-1506	8	6	2	885	-882
-13	2	2	347	-334	-12	3	2	161	179	-5	4	2	1733	1758	0	5	2	725	-729	9	6	2	405	-400
-12	2	2	1291	-1337	-11	3	2	1153	-1163	-4	4	2	139	-112	1	5	2	1487	-1508	10	6	2	570	-593
-11	2	2	1421	1439	-10	3	2	1081	-1064	-3	4	2	1385	-1383	2	5	2	586	544	11	6	2	699	-692
-9	2	2	1697	1708	-9	3	2	1276	1285	-2	4	2	172	171	3	5	2	790	739	12	6	2	790	784
-8	2	2	1603	1599	-8	3	2	643	618	-1	4	2	1559	-1596	4	5	2	405	386	13	6	2	455	440
-7	2	2	599	-575	-7	3	2	1893	1920	0	4	2	160	137	5	5	2	972	940	14	6	2	503	506
-6	2	2	712	-685	-6	3	2	1081	1070	1	4	2	672	647	6	5	2	710	-674	15	6	2	599	590
-5	2	2	1994	-2062	-5	3	2	1030	-1013	2	4	2	310	286	7	5	2	385	-364	16	6	2	507	-516
-4	2	2	1204	-1178	-4	3	2	81	-29	3	4	2	1247	1250	8	5	2	141	133	17	6	2	150	14
-3	2	2	936	906	-3	3	2	1639	-1619	4	4	2	269	261	9	5	2	1450	-1434	18	6	2	178	-203
-2	2	2	492	-462	-2	3	2	607	-590	5	4	2	565	-550	10	5	2	672	656	19	6	2	402	-407
-1	2	2	334	326	-1	3	2	1247	1215	6	4	2	166	-181	11	5	2	307	301	20	6	2	357	355
0	2	2	834	822	0	3	2	592	-556	7	4	2	1624	-1662	12	5	2	129	145	21	6	2	151	-134
1	2	2	1146	-1128	1	3	2	1247	1230	8	4	2	183	191	13	5	2	1385	1396	-21	7	2	162	-156
2	2	2	834	793	2	3	2	622	623	9	4	2	456	459	14	5	2	280	-292	-19	7	2	169	-123
3	2	2	1313	-1343	3	3	2	1095	-1094	10	4	2	385	-383	15	5	2	243	-238	-18	7	2	595	594
4	2	2	1472	-1525	4	3	2	167	-167	11	4	2	1465	1477	16	5	2	238	-237	-17	7	2	255	213
5	2	2	608	599	5	3	2	2009	-2065	12	4	2	206	-217	17	5	2	769	-760	-16	7	2	252	-223
6	2	2	131	-108	6	3	2	1182	-1169	13	4	2	175	-173	20	5	2	197	226	-15	7	2	185	174
7	2	2	1617	1678	7	3	2	494	503	15	4	2	943	-944	21	5	2	509	509	-14	7	2	972	-953
8	2	2	1653	1706	8	3	2	161	-168	18	4	2	276	283	22	5	2	158	-182	-13	7	2	405	-381
9	2	2	156	139	9	3	2	1965	2032	19	4	2	943	929	-21	6	2	239	-253	-12	7	2	234	210
10	2	2	273	269	10	3	2	627	631	20	4	2	157	177	-20	6	2	515	523	-11	7	2	187	-162
11	2	2	1204	-1215	11	3	2	363	-348	21	4	2	148	-123	-19	6	2	533	538	-10	7	2	1153	1168
12	2	2	841	-818	12	3	2	557	540	23	4	2	720	-693	-18	6	2	210	-203	-9	7	2	362	359
13	2	2	319	316	13	3	2	994	-1005	-23	5	2	201	-198	-17	6	2	504	508	-7	7	2	257	255
14	2	2	653	-645	14	3	2	113	63	-22	5	2	143	165	-16	6	2	986	-974	-6	7	2	1052	-1047
15	2	2	856	848	15	3	2	201	201	-21	5	2	535	538	-15	6	2	666	-657	-5	7	2	444	-452
16	2	2	489	491	16	3	2	255	-279	-20	5	2	239	-252	-14	6	2	144	101	-4	7	2	315	-321
17	2	2	192	-187	17	3	2	783	791	-19	5	2	524	526	-13	6	2	517	-500	-3	7	2	297	-290
18	2	2	547	560	18	3	2	244	258	-18	5	2	448	-460	-12	6	2	754	728	-2	7	2	1197	1165
19	2	2	740	-731	21	3	2	790	-796	-17	5	2	972	-1000	-11	6	2	333	310	-1	7	2	363	356
20	2	2	521	-511	22	3	2	176	-202	-16	5	2	210	-216	-9	6	2	614	601	0	7	2	487	471
22	2	2	418	-417	24	3	2	233	-219	-15	5	2	603	-611	-8	6	2	718	-733	1	7	2	524	530

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(2-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	7	2	1291	-1299	-5	9	2	265	-237	0	11	2	152	98	-3	1	3	1878	1937	-2	2	3	72	68
4	7	2	262	-262	-3	9	2	248	-236	1	11	2	498	-504	-2	1	3	600	-557	-1	2	3	1305	1277
5	7	2	558	-551	-2	9	2	523	-499	2	11	2	226	-226	-1	1	3	717	-705	0	2	3	1385	-1418
6	7	2	1124	1124	-1	9	2	160	129	3	11	2	259	238	0	1	3	384	390	1	2	3	112	114
8	7	2	379	373	0	9	2	181	-164	5	11	2	414	418	1	1	3	1639	-1736	2	2	3	182	177
9	7	2	290	272	1	9	2	445	441	-23	0	3	790	826	2	1	3	936	951	3	2	3	1429	-1487
10	7	2	841	-843	2	9	2	957	963	-21	0	3	597	611	3	1	3	603	618	4	2	3	1030	1055
11	7	2	302	-303	3	9	2	115	-96	-19	0	3	914	-943	4	1	3	234	220	5	2	3	622	594
12	7	2	524	-523	4	9	2	269	285	-17	0	3	805	-821	5	1	3	1762	1866	6	2	3	1320	1308
13	7	2	271	-257	5	9	2	402	-380	-15	0	3	659	647	6	1	3	435	-455	7	2	3	1037	1058
14	7	2	614	616	6	9	2	914	-907	-13	0	3	798	794	7	1	3	769	-776	8	2	3	719	-734
16	7	2	379	378	7	9	2	197	164	-11	0	3	1081	-1058	8	1	3	914	-907	9	2	3	588	-599
17	7	2	221	225	8	9	2	313	-311	-9	0	3	1349	-1268	9	1	3	1429	-1452	10	2	3	805	-793
18	7	2	490	-477	9	9	2	165	157	-7	0	3	1313	1220	10	1	3	151	181	11	2	3	877	-881
19	7	2	183	196	10	9	2	447	444	-5	0	3	2074	2068	11	1	3	426	422	12	2	3	682	673
20	7	2	219	-248	11	9	2	185	-178	-3	0	3	1110	-1105	12	1	3	479	488	13	2	3	124	-126
-18	8	2	161	102	12	9	2	307	303	-1	0	3	2038	-2179	13	1	3	1073	1101	14	2	3	226	228
-16	8	2	526	512	13	9	2	179	-219	1	0	3	943	951	14	1	3	661	-649	15	2	3	769	786
-14	8	2	135	-126	14	9	2	357	-356	3	0	3	2437	2745	15	1	3	162	152	16	2	3	747	-740
-12	8	2	1059	-1058	-13	10	2	295	315	5	0	3	892	-931	16	1	3	163	-147	18	2	3	453	-442
-9	8	2	131	86	-12	10	2	402	399	7	0	3	1690	-1730	17	1	3	1037	-1024	19	2	3	674	-675
-8	8	2	1139	1141	-11	10	2	344	-349	9	0	3	121	103	18	1	3	411	413	20	2	3	373	357
-4	8	2	701	-700	-9	10	2	382	-389	11	0	3	1472	1497	19	1	3	121	-98	21	2	3	132	69
-3	8	2	163	165	-8	10	2	490	-508	13	0	3	133	-84	20	1	3	245	260	22	2	3	524	533
-1	8	2	117	113	-7	10	2	448	444	15	0	3	1378	-1378	21	1	3	653	625	23	2	3	463	462
0	8	2	834	829	-6	10	2	152	-122	17	0	3	157	-39	22	1	3	131	-104	-24	3	3	189	-207
1	8	2	176	-185	-5	10	2	300	301	19	0	3	878	863	24	1	3	163	-179	-22	3	3	516	-505
2	8	2	301	325	-4	10	2	488	492	23	0	3	458	-463	-25	2	3	308	305	-21	3	3	220	-256
4	8	2	1240	-1239	-3	10	2	352	-366	-25	1	3	460	-469	-24	2	3	450	-451	-18	3	3	656	663
5	8	2	160	149	-2	10	2	149	148	-23	1	3	379	-399	-23	2	3	529	-519	-17	3	3	398	394
6	8	2	525	-560	-1	10	2	457	-453	-22	1	3	404	406	-21	2	3	211	-226	-16	3	3	120	116
8	8	2	986	977	0	10	2	521	-535	-21	1	3	928	950	-20	2	3	700	701	-15	3	3	383	390
9	8	2	133	105	1	10	2	228	213	-19	1	3	511	542	-19	2	3	725	744	-14	3	3	1349	-1364
10	8	2	420	441	3	10	2	623	637	-18	1	3	426	-444	-18	2	3	123	101	-13	3	3	273	-271
11	8	2	127	-36	4	10	2	506	501	-17	1	3	921	-945	-17	2	3	422	430	-12	3	3	105	27
12	8	2	616	-614	5	10	2	131	-115	-16	1	3	186	198	-16	2	3	914	-933	-11	3	3	732	-724
14	8	2	306	-323	7	10	2	436	-435	-15	1	3	564	-563	-15	2	3	568	-569	-10	3	3	1697	1661
16	8	2	450	457	8	10	2	244	-263	-14	1	3	548	554	-14	2	3	297	284	-9	3	3	341	317
18	8	2	300	351	9	10	2	161	157	-13	1	3	592	592	-13	2	3	1160	-1149	-8	3	3	165	131
-15	9	2	160	169	10	10	2	170	-185	-12	1	3	508	-508	-12	2	3	1472	1434	-7	3	3	370	388
-14	9	2	484	503	11	10	2	283	287	-11	1	3	1371	1300	-11	2	3	848	801	-6	3	3	1668	-1636
-13	9	2	189	-156	12	10	2	234	206	-10	1	3	776	-750	-9	2	3	1102	1060	-5	3	3	994	-927
-12	9	2	129	-70	-7	11	2	354	-368	-9	1	3	1262	-1196	-8	2	3	1639	-1600	-4	3	3	315	-303
-11	9	2	354	-360	-6	11	2	199	-187	-8	1	3	848	-795	-7	2	3	1342	-1353	-3	3	3	276	-284
-10	9	2	986	-996	-5	11	2	347	350	-7	1	3	1980	-1918	-6	2	3	516	-525	-2	3	3	1610	1589
-9	9	2	261	246	-3	11	2	489	496	-6	1	3	790	757	-5	2	3	783	-750	-1	3	3	267	260
-7	9	2	309	304	-2	11	2	284	251	-5	1	3	1320	1275	-4	2	3	943	933	0	3	3	812	769
-6	9	2	702	708	-1	11	2	356	-348	-4	1	3	790	765	-3	2	3	732	756	1	3	3	965	938

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(2-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	3	3	115	97	11	4	3	127	20	20	5	3	353	362	-11	7	3	732	728	-13	9	3	398	-403
4	3	3	1059	-1038	12	4	3	1204	-1217	21	5	3	232	-227	-10	7	3	402	369	-12	9	3	120	-87
5	3	3	863	-853	14	4	3	651	-639	-21	6	3	236	260	-9	7	3	333	-325	-11	9	3	577	-612
6	3	3	2038	2122	16	4	3	689	679	-20	6	3	450	466	-7	7	3	972	-1010	-10	9	3	421	439
7	3	3	421	424	18	4	3	411	406	-19	6	3	478	-498	-6	7	3	404	-408	-9	9	3	590	594
8	3	3	848	863	19	4	3	137	-73	-17	6	3	389	-383	-5	7	3	564	549	-7	9	3	661	684
9	3	3	492	487	20	4	3	398	-379	-16	6	3	812	-789	-4	7	3	112	-128	-6	9	3	347	-361
10	3	3	1189	-1205	22	4	3	470	-462	-15	6	3	610	594	-3	7	3	1037	1057	-5	9	3	427	-423
11	3	3	110	-82	-23	5	3	149	47	-14	6	3	189	195	-2	7	3	422	428	-4	9	3	120	93
12	3	3	640	-635	-22	5	3	472	469	-13	6	3	498	523	-1	7	3	670	-656	-3	9	3	395	-386
13	3	3	379	-359	-21	5	3	297	-298	-12	6	3	697	728	0	7	3	102	89	-2	9	3	263	246
14	3	3	682	693	-20	5	3	127	-57	-11	6	3	436	-423	1	7	3	1124	-1110	-1	9	3	282	275
15	3	3	116	-102	-19	5	3	204	-215	-10	6	3	163	-161	2	7	3	445	-426	0	9	3	133	120
16	3	3	534	539	-18	5	3	957	-972	-9	6	3	381	-387	3	7	3	443	430	1	9	3	590	608
17	3	3	333	321	-17	5	3	405	441	-8	6	3	602	-604	4	7	3	117	-113	2	9	3	351	-342
18	3	3	484	-472	-15	5	3	525	516	-7	6	3	507	500	5	7	3	1044	1037	3	9	3	356	-341
20	3	3	577	-577	-14	5	3	1182	1204	-6	6	3	371	-383	6	7	3	335	318	4	9	3	323	-317
21	3	3	392	-384	-13	5	3	165	-180	-5	6	3	856	851	7	7	3	234	-234	5	9	3	863	-879
22	3	3	375	345	-12	5	3	118	-25	-4	6	3	1001	985	8	7	3	165	161	6	9	3	334	341
23	3	3	157	15	-11	5	3	400	-398	-3	6	3	754	-715	9	7	3	885	-888	7	9	3	227	226
-24	4	3	507	499	-10	5	3	892	-885	-2	6	3	397	403	10	7	3	289	-281	8	9	3	149	144
-22	4	3	152	-113	-9	5	3	367	357	-1	6	3	1269	-1265	13	7	3	725	727	9	9	3	517	515
-20	4	3	672	-669	-8	5	3	180	-140	0	6	3	914	-932	16	7	3	265	230	10	9	3	206	-192
-19	4	3	111	22	-7	5	3	287	270	1	6	3	488	456	17	7	3	526	-542	13	9	3	338	-341
-17	4	3	292	299	-6	5	3	1255	1272	2	6	3	307	-295	-17	8	3	283	265	-11	10	3	198	-230
-16	4	3	1284	1314	-5	5	3	534	-523	3	6	3	761	749	-15	8	3	464	-459	-9	10	3	362	-341
-15	4	3	134	136	-4	5	3	418	421	4	6	3	532	520	-13	8	3	577	-612	-8	10	3	533	551
-12	4	3	1342	-1387	-3	5	3	870	-853	5	6	3	350	-326	-12	8	3	164	122	-7	10	3	272	276
-10	4	3	193	-178	-2	5	3	2031	-1990	6	6	3	410	409	-11	8	3	769	785	-6	10	3	160	56
-9	4	3	207	-203	-1	5	3	93	67	7	6	3	606	-596	-10	8	3	128	174	-5	10	3	365	377
-8	4	3	1349	1339	0	5	3	394	-390	8	6	3	543	-522	-9	8	3	856	905	-4	10	3	460	-453
-7	4	3	252	-258	1	5	3	706	673	10	6	3	580	-593	-8	8	3	142	-123	-3	10	3	175	-223
-6	4	3	395	384	2	5	3	1218	1199	11	6	3	907	937	-7	8	3	591	-605	-1	10	3	375	-382
-5	4	3	130	-107	4	5	3	335	312	12	6	3	790	765	-5	8	3	613	-642	0	10	3	418	405
-4	4	3	1973	-1964	5	5	3	244	-229	13	6	3	158	144	-3	8	3	228	225	1	10	3	198	212
-2	4	3	708	-680	6	5	3	627	-626	14	6	3	421	418	-2	8	3	151	-129	2	10	3	277	277
-1	4	3	202	185	7	5	3	431	443	15	6	3	656	-668	-1	8	3	709	706	3	10	3	432	430
0	4	3	1900	1928	8	5	3	611	-615	16	6	3	405	-402	0	8	3	112	107	4	10	3	497	-499
1	4	3	289	293	9	5	3	463	473	18	6	3	253	-286	1	8	3	371	-358	6	10	3	278	-265
2	4	3	582	586	10	5	3	928	915	19	6	3	352	340	3	8	3	1102	-1133	7	10	3	406	-402
3	4	3	220	-211	11	5	3	213	-205	20	6	3	136	139	5	8	3	415	386	8	10	3	431	445
4	4	3	1204	-1204	12	5	3	754	754	-19	7	3	284	289	6	8	3	125	133	10	10	3	152	176
5	4	3	111	118	13	5	3	483	-502	-18	7	3	287	269	7	8	3	986	990	-2	11	3	570	-563
6	4	3	769	-743	14	5	3	776	-783	-17	7	3	545	-543	9	8	3	215	-208	0	11	3	225	-206
7	4	3	147	-140	15	5	3	172	-183	-15	7	3	389	-390	11	8	3	528	-537	1	11	3	154	-125
8	4	3	1334	1320	16	5	3	517	-540	-14	7	3	249	-250	15	8	3	516	517	2	11	3	462	452
9	4	3	108	-117	17	5	3	331	315	-13	7	3	479	483	-15	9	3	278	288	-24	0	4	542	577

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(2-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-20	0	4	1313	-1355	6	1	4	1110	-1147	10	2	4	535	-528	18	3	4	175	-174	-10	5	4	309	283
-16	0	4	1044	1027	7	1	4	474	-467	11	2	4	776	791	21	3	4	679	652	-9	5	4	354	367
-12	0	4	928	-861	8	1	4	754	-745	12	2	4	574	573	22	3	4	163	178	-8	5	4	195	-180
-10	0	4	338	-306	9	1	4	732	740	14	2	4	570	572	-23	4	4	403	-432	-7	5	4	1001	992
-8	0	4	2415	2359	10	1	4	1088	1106	15	2	4	593	-596	-22	4	4	186	178	-6	5	4	547	-531
-6	0	4	608	573	11	1	4	118	145	16	2	4	226	-218	-21	4	4	307	-330	-5	5	4	513	-491
-4	0	4	2422	-2495	12	1	4	805	814	18	2	4	444	-452	-19	4	4	462	466	-4	5	4	181	-143
-2	0	4	747	-703	13	1	4	331	-332	19	2	4	536	548	-17	4	4	677	681	-3	5	4	1501	-1491
2	0	4	497	465	14	1	4	783	-797	20	2	4	299	257	-15	4	4	819	-809	-2	5	4	668	646
4	0	4	1211	-1208	15	1	4	245	237	22	2	4	268	268	-14	4	4	273	-271	-1	5	4	696	685
6	0	4	1059	-1064	16	1	4	677	-675	-23	3	4	298	-285	-13	4	4	1189	-1192	0	5	4	685	671
8	0	4	1414	1447	17	1	4	355	335	-22	3	4	139	-190	-11	4	4	856	865	1	5	4	1400	1361
10	0	4	936	939	18	1	4	420	439	-21	3	4	358	362	-10	4	4	301	-278	2	5	4	381	-364
12	0	4	812	-844	20	1	4	556	553	-19	3	4	487	500	-9	4	4	892	885	3	5	4	300	-290
14	0	4	776	-803	21	1	4	236	-222	-18	3	4	285	296	-8	4	4	175	-149	4	5	4	311	-293
16	0	4	507	521	22	1	4	292	-287	-17	3	4	658	-634	-7	4	4	598	-579	5	5	4	819	-818
18	0	4	645	656	-24	2	4	424	-448	-16	3	4	347	-357	-6	4	4	277	271	6	5	4	366	351
20	0	4	286	-313	-23	2	4	302	320	-15	3	4	1059	-1049	-5	4	4	1052	-1016	8	5	4	161	136
22	0	4	500	-487	-21	2	4	288	296	-14	3	4	643	-618	-3	4	4	686	646	9	5	4	943	973
-23	1	4	193	193	-20	2	4	515	536	-13	3	4	1015	980	-2	4	4	489	462	10	5	4	431	-431
-22	1	4	863	877	-19	2	4	345	-349	-12	3	4	263	-245	-1	4	4	1828	1857	11	5	4	135	-113
-21	1	4	228	-243	-18	2	4	241	-246	-11	3	4	1371	1358	0	4	4	210	197	12	5	4	490	-491
-20	1	4	128	-66	-17	2	4	552	-548	-10	3	4	545	547	1	4	4	552	-538	13	5	4	986	-991
-19	1	4	279	-284	-16	2	4	616	-612	-9	3	4	856	-834	2	4	4	215	-201	14	5	4	250	264
-18	1	4	1073	-1112	-15	2	4	769	742	-8	3	4	384	390	3	4	4	1668	-1690	16	5	4	361	353
-17	1	4	346	353	-13	2	4	761	726	-7	3	4	1015	-1011	4	4	4	168	-152	17	5	4	503	507
-16	1	4	281	-270	-12	2	4	907	852	-6	3	4	196	-180	5	4	4	369	367	-20	6	4	476	-472
-15	1	4	104	91	-11	2	4	921	-894	-5	3	4	347	330	6	4	4	107	-65	-19	6	4	281	-285
-14	1	4	928	883	-10	2	4	363	348	-3	3	4	1240	1234	7	4	4	1044	1039	-18	6	4	114	102
-13	1	4	493	-448	-9	2	4	1001	-951	-2	3	4	479	454	8	4	4	199	-173	-17	6	4	443	-454
-12	1	4	324	309	-8	2	4	1385	-1356	-1	3	4	436	-443	9	4	4	154	-138	-16	6	4	583	587
-11	1	4	340	-328	-7	2	4	138	99	0	3	4	231	216	11	4	4	1081	-1077	-15	6	4	309	314
-10	1	4	1342	-1285	-6	2	4	199	163	1	3	4	1487	-1521	13	4	4	135	-114	-13	6	4	305	317
-9	1	4	416	388	-5	2	4	1189	1178	2	3	4	505	-501	15	4	4	957	957	-12	6	4	607	-618
-8	1	4	483	-451	-4	2	4	1349	1341	3	3	4	381	381	17	4	4	150	160	-11	6	4	590	-600
-7	1	4	914	873	-3	2	4	83	72	4	3	4	448	-436	19	4	4	591	-590	-10	6	4	410	-419
-6	1	4	2190	2215	-2	2	4	440	414	5	3	4	1334	1357	20	4	4	157	-10	-9	6	4	293	-299
-5	1	4	109	-41	-1	2	4	1110	-1096	6	3	4	419	435	21	4	4	137	-135	-8	6	4	783	790
-4	1	4	549	524	0	2	4	928	-940	7	3	4	148	-131	-22	5	4	220	-228	-7	6	4	525	522
-3	1	4	834	-789	1	2	4	957	931	8	3	4	271	255	-21	5	4	374	-381	-6	6	4	291	299
-2	1	4	1545	-1567	2	2	4	1327	-1336	9	3	4	965	-999	-19	5	4	457	-468	-5	6	4	754	774
-1	1	4	566	554	3	2	4	1748	1803	10	3	4	368	-362	-18	5	4	302	308	-4	6	4	1044	-1044
0	1	4	664	-673	4	2	4	1030	1062	11	3	4	109	70	-17	5	4	585	561	-3	6	4	241	-239
1	1	4	336	331	5	2	4	870	-863	12	3	4	232	-228	-16	5	4	168	195	-2	6	4	344	-331
2	1	4	921	940	6	2	4	1001	988	13	3	4	754	758	-15	5	4	689	711	-1	6	4	1124	-1114
3	1	4	350	-364	7	2	4	1371	-1404	14	3	4	142	124	-14	5	4	392	-409	0	6	4	870	847
4	1	4	661	669	8	2	4	1153	-1142	16	3	4	278	274	-13	5	4	706	-716	1	6	4	263	252
5	1	4	754	-762	9	2	4	241	-239	17	3	4	841	-812	-11	5	4	732	-732	2	6	4	445	430

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(2-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	6	4	754	729	-8	8	4	943	-985	6	10	4	269	-256	5	1	5	1298	-1313	9	2	5	257	270
4	6	4	485	-473	-7	8	4	163	-176	7	10	4	329	351	6	1	5	422	412	10	2	5	550	564
5	6	4	131	-98	-6	8	4	219	-242	-23	0	5	415	-437	7	1	5	102	-9	11	2	5	668	672
6	6	4	389	-378	-4	8	4	687	681	-21	0	5	723	-740	8	1	5	490	466	12	2	5	338	-356
7	6	4	616	-595	-2	8	4	208	230	-19	0	5	740	741	9	1	5	1305	1315	14	2	5	458	-444
8	6	4	603	601	0	8	4	683	-670	-17	0	5	921	918	10	1	5	194	-193	15	2	5	501	-487
10	6	4	426	436	2	8	4	491	-512	-15	0	5	682	-656	11	1	5	104	111	16	2	5	348	352
11	6	4	706	691	3	8	4	128	106	-13	0	5	481	-452	12	1	5	326	-324	17	2	5	236	-219
12	6	4	616	-608	4	8	4	921	944	-11	0	5	577	550	13	1	5	776	-769	18	2	5	439	443
13	6	4	131	18	5	8	4	117	113	-9	0	5	1182	1123	14	1	5	292	305	19	2	5	395	395
14	6	4	409	-422	6	8	4	612	623	-7	0	5	601	-611	15	1	5	224	-219	20	2	5	194	-173
15	6	4	600	-582	8	8	4	632	-624	-5	0	5	2299	-2339	16	1	5	128	128	-22	3	5	452	469
16	6	4	329	330	10	8	4	387	-407	-3	0	5	368	394	17	1	5	545	558	-21	3	5	147	62
18	6	4	245	232	11	8	4	143	-8	-1	0	5	1458	1481	18	1	5	180	-184	-19	3	5	181	179
-18	7	4	505	-525	12	8	4	313	294	3	0	5	1066	-1052	19	1	5	154	139	-18	3	5	660	-652
-17	7	4	165	49	14	8	4	292	310	5	0	5	177	200	20	1	5	260	-236	-17	3	5	318	-300
-15	7	4	353	-351	-11	9	4	249	258	7	0	5	1472	1498	21	1	5	454	-475	-16	3	5	265	-208
-14	7	4	708	739	-10	9	4	611	646	11	0	5	1392	-1392	-23	2	5	236	235	-15	3	5	229	-230
-12	7	4	170	199	-9	9	4	159	-160	13	0	5	152	-71	-22	2	5	141	-50	-14	3	5	1313	1286
-10	7	4	950	-971	-8	9	4	165	178	15	0	5	708	721	-21	2	5	380	367	-13	3	5	365	339
-9	7	4	381	-387	-7	9	4	318	-339	19	0	5	501	-511	-20	2	5	505	-488	-12	3	5	371	348
-8	7	4	402	-428	-6	9	4	579	-592	21	0	5	184	-152	-19	2	5	321	-310	-11	3	5	526	500
-7	7	4	245	-247	-5	9	4	150	142	-23	1	5	357	386	-17	2	5	538	-526	-10	3	5	1247	-1227
-6	7	4	870	910	-4	9	4	194	-223	-22	1	5	211	-247	-16	2	5	637	620	-9	3	5	129	121
-4	7	4	241	243	-3	9	4	260	233	-21	1	5	516	-509	-15	2	5	486	462	-8	3	5	302	-296
-3	7	4	364	354	-2	9	4	464	470	-19	1	5	776	-775	-14	2	5	219	204	-7	3	5	542	-517
-2	7	4	892	-886	-1	9	4	132	-49	-18	1	5	381	397	-13	2	5	776	757	-6	3	5	914	888
-1	7	4	125	141	0	9	4	265	259	-17	1	5	648	612	-12	2	5	783	-744	-5	3	5	198	186
1	7	4	255	-235	1	9	4	331	-331	-16	1	5	197	188	-11	2	5	379	-360	-4	3	5	461	446
2	7	4	819	814	2	9	4	622	-633	-15	1	5	769	741	-10	2	5	335	-315	-3	3	5	453	425
3	7	4	201	160	4	9	4	364	-398	-14	1	5	423	-401	-9	2	5	870	-843	-2	3	5	1102	-1106
4	7	4	381	390	5	9	4	418	422	-13	1	5	484	-445	-8	2	5	928	913	-1	3	5	408	-409
5	7	4	269	253	6	9	4	600	594	-12	1	5	278	-255	-7	2	5	310	288	0	3	5	870	-862
6	7	4	667	-658	8	9	4	407	391	-11	1	5	914	-878	-6	2	5	465	451	1	3	5	687	-677
7	7	4	184	-202	9	9	4	249	-271	-10	1	5	352	363	-5	2	5	870	856	2	3	5	1276	1317
8	7	4	596	-602	10	9	4	300	-297	-9	1	5	776	735	-4	2	5	965	-936	4	3	5	716	731
9	7	4	297	-287	11	9	4	151	104	-8	1	5	429	420	-3	2	5	445	-416	5	3	5	445	436
10	7	4	511	519	-9	10	4	289	292	-7	1	5	1349	1344	-2	2	5	691	-664	6	3	5	702	-721
12	7	4	490	504	-8	10	4	334	339	-6	1	5	640	-609	-1	2	5	994	-1033	7	3	5	111	-26
13	7	4	273	252	-7	10	4	273	-272	-5	1	5	638	-654	0	2	5	1030	1022	8	3	5	569	-570
14	7	4	370	-372	-5	10	4	389	-417	-4	1	5	323	-324	1	2	5	186	188	9	3	5	267	-258
16	7	4	359	-373	-4	10	4	387	-402	-3	1	5	1407	-1412	2	2	5	568	567	10	3	5	346	351
17	7	4	193	-176	-1	10	4	423	428	-2	1	5	576	570	3	2	5	1131	1144	11	3	5	122	134
-16	8	4	470	-481	0	10	4	334	337	-1	1	5	231	204	4	2	5	776	-775	12	3	5	710	700
-15	8	4	143	124	1	10	4	133	-36	0	1	5	97	69	5	2	5	173	-179	13	3	5	339	361
-14	8	4	155	-15	2	10	4	205	186	1	1	5	1037	1035	6	2	5	769	-784	14	3	5	479	-503
-12	8	4	754	789	3	10	4	393	-404	2	1	5	615	-620	7	2	5	921	-938	15	3	5	122	-10

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(2-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
17	3	5	250	-246	-5	5	5	249	261	13	6	5	148	-28	-9	9	5	183	-198	-6	1	6	1204	-1197
18	3	5	410	401	-4	5	5	555	-552	14	6	5	329	-337	-7	9	5	468	-505	-5	1	6	224	202
19	3	5	160	-101	-3	5	5	495	495	15	6	5	388	403	-6	9	5	271	279	-4	1	6	914	-891
20	3	5	424	417	-2	5	5	928	925	16	6	5	147	149	-5	9	5	191	208	-3	1	6	493	478
-20	4	5	488	479	-1	5	5	121	-82	-17	7	5	339	334	-4	9	5	205	177	-2	1	6	1037	1050
-17	4	5	154	-173	0	5	5	562	566	-16	7	5	220	-209	-3	9	5	490	526	-1	1	6	124	-87
-16	4	5	812	-803	1	5	5	551	-552	-15	7	5	409	409	-2	9	5	194	-187	0	1	6	754	750
-15	4	5	250	-228	2	5	5	841	-822	-14	7	5	177	184	-1	9	5	166	-135	1	1	6	359	-342
-14	4	5	231	-220	4	5	5	486	-484	-13	7	5	404	-401	0	9	5	150	-163	2	1	6	740	-743
-13	4	5	125	126	5	5	5	389	381	-11	7	5	630	-654	1	9	5	506	-555	4	1	6	557	-560
-12	4	5	1204	1231	6	5	5	500	489	-10	7	5	430	-433	2	9	5	191	170	5	1	6	430	445
-10	4	5	456	445	8	5	5	556	563	-9	7	5	380	381	4	9	5	158	169	6	1	6	732	746
-8	4	5	1066	-1062	9	5	5	363	-349	-8	7	5	227	219	5	9	5	545	568	7	1	6	100	96
-7	4	5	209	201	10	5	5	513	-521	-7	7	5	790	832	6	9	5	197	-179	8	1	6	754	738
-6	4	5	305	-302	12	5	5	703	-700	-6	7	5	321	349	7	9	5	147	-39	9	1	6	434	-421
-5	4	5	136	64	13	5	5	292	285	-5	7	5	348	-336	-20	0	6	841	838	10	1	6	563	-568
-4	4	5	1037	1021	14	5	5	484	494	-4	7	5	290	281	-18	0	6	278	268	12	1	6	740	-722
-3	4	5	300	296	15	5	5	175	167	-3	7	5	669	-670	-16	0	6	783	-761	13	1	6	234	219
-2	4	5	587	585	16	5	5	557	539	-1	7	5	227	185	-14	0	6	290	-297	14	1	6	276	279
0	4	5	1284	-1296	17	5	5	165	-175	0	7	5	405	-403	-12	0	6	526	512	16	1	6	458	450
1	4	5	290	-284	18	5	5	255	-237	1	7	5	740	744	-10	0	6	349	341	17	1	6	209	-203
2	4	5	994	-975	-19	6	5	281	289	2	7	5	238	230	-8	0	6	1059	-1036	18	1	6	142	-131
3	4	5	108	71	-17	6	5	293	314	4	7	5	141	109	-6	0	6	812	-789	-21	2	6	191	-201
4	4	5	1008	1008	-16	6	5	350	356	5	7	5	856	-858	-4	0	6	1334	1334	-20	2	6	387	-387
5	4	5	444	-452	-15	6	5	368	-377	6	7	5	392	-389	-2	0	6	965	929	-19	2	6	373	382
6	4	5	769	769	-13	6	5	470	-462	9	7	5	693	707	2	0	6	491	-498	-18	2	6	191	-209
8	4	5	683	-691	-12	6	5	490	-495	10	7	5	133	140	4	0	6	613	589	-17	2	6	541	526
9	4	5	298	285	-11	6	5	255	249	12	7	5	138	162	6	0	6	805	789	-16	2	6	684	677
10	4	5	524	-562	-10	6	5	137	-120	13	7	5	504	-504	8	0	6	812	-820	-15	2	6	322	-312
11	4	5	127	73	-9	6	5	643	666	-14	8	5	152	-77	10	0	6	943	-913	-14	2	6	123	119
12	4	5	534	545	-8	6	5	714	728	-13	8	5	476	491	12	0	6	524	508	-13	2	6	878	-870
14	4	5	648	641	-7	6	5	114	-90	-11	8	5	306	-281	14	0	6	637	629	-12	2	6	848	-832
16	4	5	350	-342	-6	6	5	339	347	-10	8	5	227	-216	16	0	6	271	-267	-10	2	6	302	-277
17	4	5	165	-66	-5	6	5	740	-737	-9	8	5	589	-625	18	0	6	411	-415	-9	2	6	754	756
18	4	5	540	-526	-4	6	5	698	-693	-7	8	5	230	236	-21	1	6	185	175	-8	2	6	647	643
-19	5	5	215	206	-3	6	5	260	252	-6	8	5	181	190	-20	1	6	206	-206	-7	2	6	265	-257
-18	5	5	561	526	-2	6	5	387	-399	-5	8	5	629	652	-19	1	6	144	170	-6	2	6	476	489
-16	5	5	141	122	-1	6	5	754	735	-3	8	5	178	-187	-18	1	6	783	776	-5	2	6	754	-752
-15	5	5	317	-305	0	6	5	582	578	-2	8	5	136	85	-17	1	6	331	-298	-4	2	6	521	-531
-14	5	5	754	-764	2	6	5	271	281	-1	8	5	629	-631	-16	1	6	189	197	-3	2	6	344	346
-13	5	5	146	123	3	6	5	701	-685	1	8	5	225	203	-15	1	6	375	-365	-2	2	6	572	-566
-12	5	5	167	-191	4	6	5	632	-639	2	8	5	134	8	-14	1	6	790	-777	-1	2	6	827	821
-11	5	5	435	435	6	6	5	284	-287	3	8	5	740	762	-12	1	6	100	-78	0	2	6	683	658
-10	5	5	921	941	7	6	5	608	618	7	8	5	717	-733	-11	1	6	481	470	1	2	6	89	-70
-9	5	5	278	-284	8	6	5	472	474	8	8	5	149	-24	-10	1	6	798	774	2	2	6	552	544
-8	5	5	329	321	10	6	5	414	423	9	8	5	141	-26	-9	1	6	170	-165	3	2	6	790	-808
-7	5	5	344	-348	11	6	5	590	-590	11	8	5	438	457	-8	1	6	523	502	4	2	6	542	-534
-6	5	5	769	-772	12	6	5	297	-290	-10	9	5	257	-277	-7	1	6	446	-441	6	2	6	433	-433

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(2-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
7	2	6	561	566	-6	4	6	143	-137	-7	6	6	316	-321	2	8	6	374	399	10	1	7	202	176
8	2	6	313	325	-5	4	6	841	838	-6	6	6	400	-415	4	8	6	464	-468	11	1	7	218	-194
9	2	6	207	206	-2	4	6	266	-267	-5	6	6	658	-679	5	8	6	138	-130	12	1	7	242	249
10	2	6	358	370	-1	4	6	1073	-1109	-4	6	6	518	509	6	8	6	381	-397	13	1	7	522	519
11	2	6	511	-516	0	4	6	154	-113	-3	6	6	132	-24	8	8	6	332	315	15	1	7	212	192
12	2	6	239	-229	2	4	6	159	141	-2	6	6	229	248	-4	9	6	210	220	-18	2	7	145	35
14	2	6	425	-419	3	4	6	1102	1113	-1	6	6	472	471	-3	9	6	219	-216	-17	2	7	437	437
15	2	6	410	415	4	4	6	119	26	0	6	6	553	-540	-2	9	6	468	-442	-16	2	7	503	-505
18	2	6	392	374	7	4	6	714	-728	1	6	6	134	16	0	9	6	292	-311	-15	2	7	242	-244
-19	3	6	339	-319	11	4	6	660	687	2	6	6	284	-286	1	9	6	239	210	-14	2	7	380	-387
-18	3	6	262	-232	13	4	6	139	100	3	6	6	326	-333	-19	0	7	219	-231	-13	2	7	503	-485
-17	3	6	348	331	15	4	6	629	-633	4	6	6	441	448	-17	0	7	691	-660	-12	2	7	466	474
-15	3	6	732	720	-18	5	6	183	-196	6	6	6	443	442	-15	0	7	279	281	-11	2	7	320	313
-14	3	6	437	418	-17	5	6	231	-224	7	6	6	445	470	-13	0	7	827	794	-10	2	7	442	424
-13	3	6	252	-286	-15	5	6	439	-454	8	6	6	305	-316	-11	0	7	240	-228	-9	2	7	496	499
-11	3	6	1052	-1046	-14	5	6	279	284	10	6	6	372	-402	-9	0	7	986	-999	-8	2	7	432	-447
-10	3	6	371	-348	-13	5	6	255	272	11	6	6	440	-434	-7	0	7	141	176	-6	2	7	220	-202
-9	3	6	367	340	-11	5	6	720	754	12	6	6	252	222	-5	0	7	1197	1209	-5	2	7	585	-589
-8	3	6	273	-267	-10	5	6	401	-392	13	6	6	149	-120	-1	0	7	834	-842	-4	2	7	510	500
-7	3	6	673	664	-9	5	6	397	-401	-14	7	6	437	-460	3	0	7	617	631	-2	2	7	460	456
-6	3	6	154	153	-8	5	6	276	-269	-12	7	6	160	-163	7	0	7	761	-757	-1	2	7	704	707
-5	3	6	305	-289	-7	5	6	907	-915	-10	7	6	495	499	9	0	7	309	-282	0	2	7	436	-450
-4	3	6	104	89	-6	5	6	387	375	-9	7	6	299	302	11	0	7	740	708	2	2	7	630	-610
-3	3	6	783	-777	-5	5	6	382	368	-8	7	6	356	392	13	0	7	252	236	3	2	7	682	-675
-2	3	6	457	-471	-4	5	6	311	306	-7	7	6	209	201	15	0	7	391	-364	4	2	7	304	327
1	3	6	1284	1306	-3	5	6	776	784	-6	7	6	513	-525	-19	1	7	505	501	5	2	7	157	-73
2	3	6	460	448	-2	5	6	238	-249	-5	7	6	199	-138	-18	1	7	350	-312	6	2	7	513	488
4	3	6	477	485	-1	5	6	150	-130	-4	7	6	402	-412	-17	1	7	179	-202	7	2	7	478	483
5	3	6	1218	-1250	0	5	6	256	-266	-3	7	6	273	-263	-15	1	7	626	-622	8	2	7	345	-344
6	3	6	132	-83	1	5	6	834	-856	-2	7	6	551	548	-14	1	7	200	222	9	2	7	199	199
8	3	6	389	-389	2	5	6	197	199	-1	7	6	174	-177	-13	1	7	241	268	10	2	7	366	-369
9	3	6	783	804	3	5	6	123	-44	0	7	6	362	347	-12	1	7	191	168	11	2	7	400	-402
10	3	6	121	75	4	5	6	115	167	1	7	6	246	237	-11	1	7	700	680	12	2	7	152	179
11	3	6	140	96	5	5	6	769	794	2	7	6	548	-522	-9	1	7	231	-221	13	2	7	198	-169
12	3	6	215	200	6	5	6	204	-184	4	7	6	517	-534	-8	1	7	181	-139	14	2	7	410	413
13	3	6	588	-597	8	5	6	179	-165	5	7	6	293	-279	-7	1	7	812	-831	15	2	7	366	358
14	3	6	178	-165	9	5	6	602	-617	6	7	6	412	406	-6	1	7	379	384	-18	3	7	487	503
15	3	6	265	-260	10	5	6	145	149	7	7	6	135	142	-4	1	7	184	166	-16	3	7	223	215
16	3	6	227	-229	12	5	6	263	259	8	7	6	511	530	-3	1	7	1023	1013	-15	3	7	246	241
17	3	6	517	515	13	5	6	519	517	9	7	6	254	234	-2	1	7	438	-427	-14	3	7	661	-662
-19	4	6	251	-276	-16	6	6	302	-313	10	7	6	284	-279	0	1	7	379	-369	-13	3	7	186	-216
-17	4	6	494	-491	-15	6	6	131	-61	-10	8	6	284	-268	1	1	7	878	-852	-12	3	7	392	-397
-15	4	6	329	337	-13	6	6	334	-348	-9	8	6	136	71	2	1	7	157	150	-11	3	7	295	-281
-13	4	6	878	891	-12	6	6	416	426	-8	8	6	495	509	4	1	7	339	343	-10	3	7	621	621
-11	4	6	392	-381	-11	6	6	269	267	-6	8	6	307	348	5	1	7	776	788	-8	3	7	456	439
-10	4	6	143	163	-10	6	6	295	311	-4	8	6	505	-506	7	1	7	132	115	-7	3	7	263	272
-9	4	6	936	-949	-9	6	6	567	578	-2	8	6	363	-376	8	1	7	278	-298	-6	3	7	611	-614
-7	4	6	154	138	-8	6	6	535	-548	0	8	6	485	476	9	1	7	747	-756	-4	3	7	479	-477

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(2-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-3	3	7	239	-240	0	5	7	363	-383	4	0	8	330	-335	6	2	8	396	364	4	5	8	170	-198
-2	3	7	661	663	1	5	7	267	270	6	0	8	577	-566	7	2	8	349	-346	5	5	8	397	-397
-1	3	7	123	108	2	5	7	418	419	8	0	8	297	339	8	2	8	152	-164	6	5	8	137	143
0	3	7	725	728	3	5	7	115	21	10	0	8	528	522	9	2	8	131	-102	-6	6	8	314	309
1	3	7	383	390	4	5	7	534	548	-15	1	8	237	260	10	2	8	322	-323	-5	6	8	398	407
2	3	7	545	-568	5	5	7	338	-346	-14	1	8	506	507	11	2	8	338	332	-4	6	8	258	-225
4	3	7	667	-656	6	5	7	386	-390	-13	1	8	178	114	-13	3	8	183	89	-2	6	8	233	-244
5	3	7	323	-314	8	5	7	588	-600	-12	1	8	297	299	-12	3	8	131	-126	-1	6	8	312	-307
6	3	7	347	369	9	5	7	257	275	-11	1	8	257	-305	-11	3	8	579	588	0	6	8	205	200
8	3	7	411	405	10	5	7	281	284	-10	1	8	514	-534	-10	3	8	220	205	2	6	8	279	245
10	3	7	290	-298	12	5	7	413	428	-9	1	8	181	-148	-8	3	8	178	158	-9	0	9	507	510
11	3	7	145	63	-13	6	7	297	313	-8	1	8	405	-435	-7	3	8	502	-524	-5	0	9	464	-464
12	3	7	375	-379	-12	6	7	269	291	-7	1	8	252	242	-6	3	8	133	-112	-1	0	9	466	498
13	3	7	231	-180	-11	6	7	164	-120	-6	1	8	465	466	-4	3	8	239	-253	3	0	9	566	-548
14	3	7	203	224	-10	6	7	162	164	-4	1	8	505	511	-3	3	8	620	631	5	0	9	191	-202
-16	4	7	500	503	-9	6	7	539	-558	-3	1	8	346	-323	0	3	8	201	218	-8	1	9	139	167
-14	4	7	292	289	-8	6	7	484	-516	-2	1	8	362	-392	1	3	8	701	-708	-7	1	9	485	507
-12	4	7	677	-676	-6	6	7	239	-231	0	1	8	524	-507	2	3	8	255	-200	-6	1	9	213	-223
-10	4	7	451	-460	-5	6	7	561	586	1	1	8	284	283	3	3	8	152	-162	-4	1	9	136	-108
-8	4	7	719	726	-4	6	7	343	359	2	1	8	371	357	4	3	8	[illegible]5	-198	-3	1	9	470	-474
-7	4	7	149	-44	-2	6	7	315	300	4	1	8	479	469	5	3	8	530	523	-2	1	9	177	152
-6	4	7	429	440	-1	6	7	371	-396	6	1	8	283	-262	7	3	8	202	164	-1	1	9	136	-113
-5	4	7	135	-32	0	6	7	144	-136	7	1	8	150	-50	9	3	8	342	-349	0	1	9	165	181
-4	4	7	529	-557	2	6	7	350	-346	8	1	8	515	-488	10	3	8	159	-76	1	1	9	490	476
-2	4	7	503	-495	3	6	7	394	402	9	1	8	220	213	-9	4	8	603	622	3	1	9	158	109
0	4	7	566	586	4	6	7	286	270	-15	2	8	169	130	-8	4	8	130	-6	4	1	9	229	-182
1	4	7	119	-13	5	6	7	168	158	-14	2	8	249	-208	-7	4	8	140	-57	5	1	9	435	-419
2	4	7	592	608	6	6	7	325	343	-13	2	8	462	448	-5	4	8	696	-687	-8	2	9	194	213
4	4	7	518	-522	7	6	7	397	-403	-12	2	8	413	427	-3	4	8	119	53	-6	2	9	220	249
6	4	7	481	-495	8	6	7	257	-262	-10	2	8	226	238	-1	4	8	571	586	-5	2	9	338	381
8	4	7	277	291	9	6	7	194	-181	-9	2	8	413	-428	2	4	8	143	20	-4	2	9	276	-285
10	4	7	379	391	-10	7	7	197	182	-8	2	8	323	-341	3	4	8	561	-574	-2	2	9	368	-375
12	4	7	197	-179	-7	7	7	547	-584	-7	2	8	149	70	5	4	8	183	-215	-1	2	9	358	-372
-15	5	7	148	125	-5	7	7	148	31	-6	2	8	345	-359	7	4	8	535	530	0	2	9	206	238
-14	5	7	329	346	-3	7	7	538	543	-5	2	8	508	500	-10	5	8	234	205	2	2	9	408	388
-12	5	7	227	224	1	7	7	484	-490	-4	2	8	225	236	-7	5	8	625	638	3	2	9	365	352
-11	5	7	281	-283	5	7	7	483	481	-3	2	8	132	-147	-6	5	8	154	-130	4	2	9	141	-88
-10	5	7	545	-567	-14	0	8	262	274	-2	2	8	421	409	-5	5	8	152	14	-6	3	9	300	301
-8	5	7	447	-443	-12	0	8	631	-639	-1	2	8	566	-562	-4	5	8	224	-232	-4	3	9	342	357
-7	5	7	305	308	-10	0	8	320	-314	0	2	8	329	-351	-3	5	8	508	-511	-3	3	9	170	184
-6	5	7	599	600	-8	0	8	661	641	1	2	8	154	-133	-1	5	8	133	-100	-2	3	9	239	-266
-5	5	7	141	93	-6	0	8	470	477	2	2	8	403	-381	0	5	8	178	154	0	3	9	353	-377
-4	5	7	474	469	-4	0	8	501	-517	3	2	8	466	472	1	5	8	373	389	1	3	9	160	-176
-3	5	7	230	-215	-2	0	8	657	-651	4	2	8	339	337	2	5	8	199	-189	2	3	9	150	193
-2	5	7	472	-474	2	0	8	619	588	5	2	8	180	174										

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(3-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	0	0	687	734	-1	3	0	626	573	3	6	0	270	257	-3	-10	1	131	141	1	-6	1	392	372
2	0	0	327	289	0	3	0	976	931	4	6	0	164	161	-2	-10	1	167	174	2	-6	1	373	352
3	0	0	750	722	1	3	0	856	807	5	6	0	151	153	-1	-10	1	177	190	3	-6	1	278	268
4	0	0	517	499	2	3	0	663	647	6	6	0	147	152	0	-10	1	200	216	4	-6	1	291	284
5	0	0	410	399	3	3	0	371	377	-6	7	0	114	127	1	-10	1	167	182	5	-6	1	225	234
6	0	0	210	212	4	3	0	207	244	-5	7	0	125	127	2	-10	1	173	182	6	-6	1	128	140
7	0	0	104	92	5	3	0	304	338	-4	7	0	191	209	3	-10	1	151	170	7	-6	1	100	98
8	0	0	98	98	6	3	0	180	205	-3	7	0	327	340	-4	-9	1	89	101	-7	-5	1	84	78
-7	1	0	111	108	7	3	0	91	97	-2	7	0	300	293	-3	-9	1	98	99	-6	-5	1	101	117
-6	1	0	170	169	-7	4	0	88	98	-1	7	0	392	400	-2	-9	1	110	119	-5	-5	1	191	215
-5	1	0	233	229	-6	4	0	137	141	0	7	0	433	418	-1	-9	1	171	173	-4	-5	1	248	260
-4	1	0	435	403	-5	4	0	161	170	1	7	0	327	310	0	-9	1	172	180	-3	-5	1	238	244
-3	1	0	375	328	-4	4	0	296	288	2	7	0	429	425	1	-9	1	123	130	-2	-5	1	175	177
-2	1	0	281	245	-3	4	0	562	525	3	7	0	342	333	2	-9	1	125	123	-1	-5	1	354	324
-1	1	0	961	855	-2	4	0	465	419	4	7	0	194	188	3	-9	1	158	176	0	-5	1	547	513
0	1	0	833	899	-1	4	0	391	352	5	7	0	174	180	4	-9	1	122	146	1	-5	1	308	287
1	1	0	483	511	0	4	0	743	680	6	7	0	136	133	-6	-8	1	89	100	2	-5	1	230	198
2	1	0	422	470	1	4	0	848	804	7	7	0	84	78	-5	-8	1	142	148	3	-5	1	218	201
3	1	0	489	518	2	4	0	551	528	-4	8	0	100	115	-4	-8	1	157	155	4	-5	1	235	227
4	1	0	439	463	3	4	0	373	363	-3	8	0	176	189	-3	-8	1	176	177	5	-5	1	217	221
5	1	0	359	360	4	4	0	358	370	-2	8	0	206	211	-2	-8	1	185	184	6	-5	1	142	138
6	1	0	203	204	5	4	0	298	321	-1	8	0	166	166	-1	-8	1	266	262	-8	-4	1	86	83
7	1	0	119	123	6	4	0	185	204	0	8	0	164	169	0	-8	1	306	302	-7	-4	1	101	113
8	1	0	101	100	7	4	0	109	111	1	8	0	215	205	1	-8	1	191	181	-6	-4	1	138	149
-8	2	0	100	101	-7	5	0	88	99	2	8	0	266	278	2	-8	1	115	115	-5	-4	1	242	268
-7	2	0	120	119	-6	5	0	99	106	3	8	0	207	212	3	-8	1	175	176	-4	-4	1	342	377
-6	2	0	140	138	-5	5	0	107	123	4	8	0	128	128	4	-8	1	163	179	-3	-4	1	433	468
-5	2	0	269	255	-4	5	0	232	234	5	8	0	122	127	5	-8	1	83	103	-2	-4	1	513	525
-4	2	0	468	442	-3	5	0	376	357	6	8	0	113	105	-6	-7	1	125	131	-1	-4	1	537	509
-3	2	0	526	461	-2	5	0	259	237	-4	9	0	108	121	-5	-7	1	167	177	0	-4	1	803	770
-2	2	0	198	170	-1	5	0	155	141	-3	9	0	128	147	-4	-7	1	206	205	1	-4	1	741	710
-1	2	0	386	319	0	5	0	352	316	-2	9	0	171	187	-3	-7	1	269	272	2	-4	1	489	437
0	2	0	780	760	1	5	0	425	384	-1	9	0	154	173	-2	-7	1	286	283	3	-4	1	317	290
1	2	0	504	467	2	5	0	395	385	0	9	0	114	120	-1	-7	1	484	459	4	-4	1	356	333
2	2	0	304	330	3	5	0	213	212	1	9	0	134	143	0	-7	1	573	554	5	-4	1	356	339
3	2	0	262	283	4	5	0	179	181	2	9	0	161	173	1	-7	1	243	236	6	-4	1	152	146
4	2	0	234	272	5	5	0	189	199	3	9	0	142	144	2	-7	1	318	302	7	-4	1	80	79
5	2	0	228	247	6	5	0	143	158	5	9	0	80	75	3	-7	1	380	385	-7	-3	1	77	70
6	2	0	172	183	7	5	0	90	107	-2	10	0	194	220	4	-7	1	229	236	-6	-3	1	129	139
7	2	0	86	98	-6	6	0	107	124	-1	10	0	165	190	5	-7	1	180	182	-5	-3	1	180	206
8	2	0	86	79	-5	6	0	158	173	0	10	0	161	181	6	-7	1	92	110	-4	-3	1	337	399
-8	3	0	89	90	-4	6	0	260	265	1	10	0	170	189	-6	-6	1	98	100	-3	-3	1	513	565
-7	3	0	130	128	-3	6	0	408	408	2	10	0	184	203	-5	-6	1	120	130	-2	-3	1	200	240
-6	3	0	160	168	-2	6	0	359	346	3	10	0	129	144	-4	-6	1	230	232	-1	-3	1	525	529
-5	3	0	336	333	-1	6	0	200	187	4	10	0	100	106	-3	-6	1	197	200	0	-3	1	998	1022
-4	3	0	478	441	0	6	0	493	463	-1	-11	1	153	165	-2	-6	1	204	205	1	-3	1	886	851
-3	3	0	567	524	1	6	0	501	472	0	-11	1	100	133	-1	-6	1	438	402	2	-3	1	635	570
-2	3	0	696	608	2	6	0	250	242	-4	-10	1	83	87	0	-6	1	386	363	3	-3	1	502	451

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(3-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
4	-3	1	522	476	4	0	1	266	242	3	3	1	528	499	-4	7	1	173	187	2	-10	2	159	170
5	-3	1	377	350	5	0	1	449	418	4	3	1	336	341	-3	7	1	215	231	3	-10	2	146	160
6	-3	1	222	213	6	0	1	293	282	5	3	1	259	267	-2	7	1	323	337	-5	-9	2	70	72
7	-3	1	137	142	7	0	1	146	161	6	3	1	155	177	-1	7	1	420	424	-4	-9	2	101	105
8	-3	1	97	93	8	0	1	93	98	7	3	1	138	152	0	7	1	305	294	-3	-9	2	104	107
-7	-2	1	97	104	-7	1	1	137	128	-6	4	1	162	168	1	7	1	365	350	-2	-9	2	96	103
-6	-2	1	116	126	-6	1	1	119	109	-5	4	1	142	136	2	7	1	432	434	-1	-9	2	126	127
-5	-2	1	173	196	-5	1	1	143	150	-4	4	1	227	228	3	7	1	306	302	0	-9	2	170	183
-4	-2	1	326	349	-4	1	1	344	335	-3	4	1	401	393	4	7	1	233	226	1	-9	2	143	158
-3	-2	1	360	400	-3	1	1	516	485	-2	4	1	464	431	5	7	1	197	190	2	-9	2	126	129
-2	-2	1	138	159	-2	1	1	471	419	-1	4	1	552	502	6	7	1	131	126	3	-9	2	116	126
-1	-2	1	173	172	-1	1	1	226	190	0	4	1	570	506	7	7	1	101	95	4	-9	2	116	130
0	-2	1	725	800	0	1	1	594	560	1	4	1	552	490	-4	8	1	83	94	5	-9	2	125	124
1	-2	1	614	582	1	1	1	938	910	2	4	1	704	664	-3	8	1	106	110	-5	-8	2	101	105
2	-2	1	453	396	2	1	1	893	827	3	4	1	596	558	-2	8	1	157	173	-4	-8	2	169	175
3	-2	1	254	237	3	1	1	321	377	4	4	1	303	297	-1	8	1	228	248	-3	-8	2	215	220
4	-2	1	321	283	4	1	1	256	280	5	4	1	254	245	0	8	1	190	191	-2	-8	2	173	173
5	-2	1	372	337	5	1	1	356	362	6	4	1	220	226	1	8	1	145	142	-1	-8	2	224	214
6	-2	1	244	227	6	1	1	278	283	7	4	1	144	158	2	8	1	208	220	0	-8	2	269	265
7	-2	1	116	123	7	1	1	154	162	-6	5	1	137	140	3	8	1	206	203	1	-8	2	235	229
8	-2	1	90	73	8	1	1	82	86	-5	5	1	132	134	4	8	1	161	171	2	-8	2	208	205
-8	-1	1	86	94	-8	2	1	98	79	-4	5	1	139	146	5	8	1	134	133	3	-8	2	170	173
-7	-1	1	134	128	-7	2	1	131	144	-3	5	1	246	244	6	8	1	98	95	4	-8	2	102	105
-6	-1	1	191	188	-6	2	1	188	180	-2	5	1	337	313	-3	9	1	110	130	5	-8	2	116	125
-5	-1	1	251	262	-5	2	1	179	175	-1	5	1	368	333	-2	9	1	157	185	6	-8	2	90	110
-4	-1	1	424	436	-4	2	1	283	277	0	5	1	272	249	-1	9	1	167	176	-6	-7	2	87	82
-3	-1	1	615	625	-3	2	1	515	474	1	5	1	237	202	0	9	1	149	172	-5	-7	2	115	116
-2	-1	1	454	473	-2	2	1	615	565	2	5	1	341	315	1	9	1	136	140	-4	-7	2	240	251
-1	-1	1	444	515	-1	2	1	447	391	3	5	1	359	337	2	9	1	120	131	-3	-7	2	303	311
0	-1	1	810	1107	0	2	1	182	181	4	5	1	235	233	3	9	1	134	138	-2	-7	2	245	234
1	-1	1	536	578	1	2	1	630	510	5	5	1	140	143	4	9	1	104	117	-1	-7	2	356	347
2	-1	1	320	304	2	2	1	699	635	6	5	1	147	152	5	9	1	100	97	0	-7	2	422	408
3	-1	1	642	559	3	2	1	307	308	7	5	1	101	112	-1	10	1	184	220	1	-7	2	488	459
4	-1	1	300	279	4	2	1	133	163	-6	6	1	149	162	0	10	1	205	235	2	-7	2	468	452
5	-1	1	299	258	5	2	1	238	261	-5	6	1	158	167	1	10	1	150	167	3	-7	2	179	179
6	-1	1	241	231	6	2	1	202	220	-4	6	1	160	172	2	10	1	141	159	4	-7	2	227	211
7	-1	1	91	96	7	2	1	99	110	-3	6	1	299	319	3	10	1	152	168	5	-7	2	254	266
8	-1	1	92	86	8	2	1	89	83	-2	6	1	404	395	4	10	1	124	136	6	-7	2	126	138
-7	0	1	155	149	-7	3	1	125	127	-1	6	1	465	453	-2	-11	2	112	119	-5	-6	2	93	122
-6	0	1	194	196	-6	3	1	187	175	0	6	1	390	364	-1	-11	2	132	140	-4	-6	2	189	202
-5	0	1	168	167	-5	3	1	214	212	1	6	1	155	133	0	-11	2	155	167	-3	-6	2	206	216
-4	0	1	449	456	-4	3	1	305	300	2	6	1	464	440	1	-11	2	138	150	-2	-6	2	236	239
-3	0	1	856	808	-3	3	1	720	690	3	6	1	428	417	-4	-10	2	101	100	-1	-6	2	233	222
-2	0	1	624	572	-2	3	1	739	665	4	6	1	131	125	-3	-10	2	121	127	0	-6	2	353	341
-1	0	1	931	964	-1	3	1	510	449	5	6	1	154	143	-2	-10	2	91	110	1	-6	2	474	447
1	0	1	383	720	0	3	1	810	741	6	6	1	125	128	-1	-10	2	191	194	2	-6	2	342	316
2	0	1	1741	1607	1	3	1	788	710	7	6	1	95	89	0	-10	2	218	230	3	-6	2	254	249
3	0	1	648	607	2	3	1	863	789	-5	7	1	111	125	1	-10	2	173	186	4	-6	2	262	261

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(3-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
5	-6	2	248	235	8	-3	2	98	87	-7	1	2	94	101	-5	4	2	157	161	2	7	2	286	275
6	-6	2	166	169	-7	-2	2	122	125	-6	1	2	173	172	-4	4	2	214	212	3	7	2	305	294
7	-6	2	89	103	-6	-2	2	131	138	-5	1	2	187	179	-3	4	2	208	205	4	7	2	305	306
-7	-5	2	83	88	-5	-2	2	113	124	-4	1	2	137	137	-2	4	2	389	370	5	7	2	206	198
-6	-5	2	104	107	-4	-2	2	199	203	-3	1	2	313	288	-1	4	2	657	611	6	7	2	113	110
-5	-5	2	117	126	-3	-2	2	391	411	-2	1	2	584	545	0	4	2	518	488	7	7	2	96	95
-4	-5	2	218	238	-2	-2	2	399	439	-1	1	2	660	611	1	4	2	367	318	-3	8	2	105	118
-3	-5	2	332	357	-1	-2	2	326	348	0	1	2	330	327	2	4	2	569	527	-2	8	2	92	112
-2	-5	2	272	268	0	-2	2	125	156	1	1	2	234	187	3	4	2	566	518	-1	8	2	156	176
-1	-5	2	224	209	1	-2	2	202	254	2	1	2	788	764	4	4	2	458	421	0	8	2	199	209
0	-5	2	251	253	2	-2	2	706	719	3	1	2	722	647	5	4	2	298	277	1	8	2	211	217
1	-5	2	420	424	3	-2	2	538	498	4	1	2	428	417	6	4	2	179	171	2	8	2	152	161
2	-5	2	423	384	4	-2	2	233	213	5	1	2	237	259	7	4	2	149	147	3	8	2	144	147
3	-5	2	182	174	5	-2	2	208	187	6	1	2	205	206	8	4	2	92	104	4	8	2	173	188
4	-5	2	173	165	6	-2	2	263	235	7	1	2	185	186	-6	5	2	102	117	5	8	2	137	143
5	-5	2	219	208	7	-2	2	183	172	8	1	2	109	125	-5	5	2	163	169	6	8	2	80	90
6	-5	2	157	151	8	-2	2	80	96	-7	2	2	101	95	-4	5	2	180	182	-2	9	2	101	112
7	-5	2	93	97	-7	-1	2	140	142	-6	2	2	179	170	-3	5	2	152	157	-1	9	2	152	171
-7	-4	2	95	83	-6	-1	2	206	200	-5	2	2	245	244	-2	5	2	230	223	0	9	2	200	231
-6	-4	2	145	153	-5	-1	2	187	187	-4	2	2	248	241	-1	5	2	401	380	1	9	2	133	141
-5	-4	2	187	215	-4	-1	2	302	314	-3	2	2	317	304	0	5	2	334	306	2	9	2	122	129
-4	-4	2	277	301	-3	-1	2	594	598	-2	2	2	528	477	1	5	2	197	176	3	9	2	116	128
-3	-4	2	489	542	-2	-1	2	637	651	-1	2	2	590	540	2	5	2	306	284	4	9	2	111	119
-2	-4	2	426	474	-1	-1	2	587	632	0	2	2	554	507	3	5	2	350	321	5	9	2	86	96
-1	-4	2	426	442	0	-1	2	437	476	1	2	2	361	300	4	5	2	206	193	0	10	2	170	196
0	-4	2	765	749	1	-1	2	248	416	2	2	2	376	350	5	5	2	204	188	1	10	2	167	191
1	-4	2	613	621	2	-1	2	968	1173	3	2	2	561	481	6	5	2	155	157	2	10	2	164	189
2	-4	2	672	616	3	-1	2	495	464	4	2	2	368	340	7	5	2	93	94	3	10	2	128	140
3	-4	2	445	425	4	-1	2	83	72	5	2	2	189	185	8	5	2	82	84	-2	-11	3	119	121
4	-4	2	302	276	5	-1	2	380	329	6	2	2	118	132	-5	6	2	164	179	-1	-11	3	125	123
5	-4	2	268	238	6	-1	2	262	241	7	2	2	152	162	-4	6	2	234	256	0	-11	3	137	152
6	-4	2	215	197	7	-1	2	152	136	8	2	2	103	114	-3	6	2	223	232	1	-11	3	121	143
7	-4	2	146	158	8	-1	2	96	100	-6	3	2	221	237	-2	6	2	233	235	-4	-10	3	97	101
-7	-3	2	107	119	-7	0	2	126	123	-5	3	2	244	239	-1	6	2	480	475	-3	-10	3	123	123
-6	-3	2	157	171	-6	0	2	172	172	-4	3	2	261	255	0	6	2	434	422	-2	-10	3	119	130
-5	-3	2	101	105	-5	0	2	222	219	-3	3	2	389	371	1	6	2	338	317	-1	-10	3	145	149
-4	-3	2	239	272	-4	0	2	359	362	-2	3	2	528	495	2	6	2	373	353	0	-10	3	124	146
-3	-3	2	391	433	-3	0	2	418	401	-1	3	2	1013	960	3	6	2	182	167	1	-10	3	213	215
-2	-3	2	444	522	-2	0	2	725	723	0	3	2	803	735	4	6	2	284	270	2	-10	3	197	209
-1	-3	2	597	641	-1	0	2	1081	1089	1	3	2	364	293	5	6	2	254	255	3	-10	3	118	144
0	-3	2	376	416	1	0	2	683	987	2	3	2	724	671	6	6	2	81	83	4	-10	3	116	120
1	-3	2	626	673	2	0	2	878	970	3	3	2	717	658	7	6	2	74	79	-4	-9	3	81	87
2	-3	2	893	861	3	0	2	455	557	4	3	2	464	413	-4	7	2	161	182	-3	-9	3	119	126
3	-3	2	606	561	4	0	2	684	605	5	3	2	260	242	-3	7	2	137	161	-2	-9	3	111	114
4	-3	2	346	324	5	0	2	404	376	6	3	2	196	199	-2	7	2	238	252	-1	-9	3	94	99
5	-3	2	359	320	6	0	2	239	211	7	3	2	144	158	-1	7	2	357	370	0	-9	3	115	120
6	-3	2	314	286	7	0	2	207	192	8	3	2	88	90	0	7	2	391	400	1	-9	3	157	158
7	-3	2	177	163	8	0	2	132	117	-6	4	2	118	126	1	7	2	356	345	2	-9	3	179	183

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [Ni(3-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	-9	3	120	121	-2	-5	3	346	363	0	-2	3	310	352	3	1	3	444	407	7	4	3	137	127
4	-9	3	79	88	-1	-5	3	379	387	1	-2	3	164	201	4	1	3	551	533	8	4	3	94	91
5	-9	3	100	107	0	-5	3	240	232	2	-2	3	336	352	5	1	3	358	333	-5	5	3	116	133
-5	-8	3	92	91	1	-5	3	210	208	3	-2	3	377	398	6	1	3	174	194	-4	5	3	206	224
-4	-8	3	144	155	2	-5	3	336	308	4	-2	3	326	341	7	1	3	158	163	-3	5	3	193	196
-3	-8	3	187	194	3	-5	3	361	359	5	-2	3	326	297	8	1	3	134	121	-2	5	3	151	151
-2	-8	3	204	213	4	-5	3	208	209	6	-2	3	193	178	-6	2	3	143	164	-1	5	3	254	243
-1	-8	3	226	226	5	-5	3	123	121	7	-2	3	143	116	-5	2	3	208	215	0	5	3	352	331
0	-8	3	193	199	6	-5	3	154	141	8	-2	3	131	121	-4	2	3	261	249	1	5	3	356	328
1	-8	3	252	231	7	-5	3	141	136	-7	-1	3	73	88	-3	2	3	306	297	2	5	3	273	248
2	-8	3	269	268	-7	-4	3	95	105	-6	-1	3	162	163	-2	2	3	312	295	3	5	3	133	127
3	-8	3	140	146	-6	-4	3	172	178	-5	-1	3	279	280	-1	2	3	597	553	4	5	3	263	251
4	-8	3	110	113	-5	-4	3	137	132	-4	-1	3	315	315	0	2	3	667	611	5	5	3	300	279
5	-8	3	143	154	-4	-4	3	215	226	-3	-1	3	247	253	1	2	3	266	233	6	5	3	104	98
6	-8	3	96	87	-3	-4	3	369	412	-2	-1	3	491	491	2	2	3	392	394	7	5	3	94	86
-6	-7	3	91	86	-2	-4	3	457	500	-1	-1	3	991	1016	3	2	3	429	384	8	5	3	96	96
-5	-7	3	116	117	-1	-4	3	687	728	0	-1	3	629	643	4	2	3	371	325	-4	6	3	198	226
-4	-7	3	162	163	0	-4	3	409	444	1	-1	3	235	320	5	2	3	307	268	-3	6	3	230	245
-3	-7	3	212	220	1	-4	3	325	368	2	-1	3	466	547	6	2	3	182	172	-2	6	3	278	286
-2	-7	3	339	344	2	-4	3	780	742	3	-1	3	346	407	7	2	3	114	123	-1	6	3	314	327
-1	-7	3	379	379	3	-4	3	539	531	4	-1	3	579	640	8	2	3	87	85	0	6	3	320	314
0	-7	3	268	257	4	-4	3	329	315	5	-1	3	303	288	-6	3	3	83	94	1	6	3	465	449
1	-7	3	419	393	5	-4	3	236	228	6	-1	3	87	52	-5	3	3	165	172	2	6	3	331	324
2	-7	3	415	407	6	-4	3	211	190	7	-1	3	195	177	-4	3	3	411	421	3	6	3	220	211
3	-7	3	318	322	7	-4	3	158	142	8	-1	3	149	138	-3	3	3	335	326	4	6	3	287	280
4	-7	3	278	276	8	-4	3	92	88	-6	0	3	155	161	-2	3	3	335	320	5	6	3	167	156
5	-7	3	141	144	-7	-3	3	83	92	-5	0	3	266	259	-1	3	3	681	653	6	6	3	128	123
6	-7	3	149	132	-6	-3	3	78	96	-4	0	3	286	271	0	3	3	680	631	7	6	3	117	124
7	-7	3	122	130	-5	-3	3	167	178	-3	0	3	277	270	1	3	3	810	738	-4	7	3	143	166
-6	-6	3	97	92	-4	-3	3	230	241	-2	0	3	633	620	2	3	3	622	597	-3	7	3	203	230
-5	-6	3	88	99	-3	-3	3	197	217	-1	0	3	818	820	3	3	3	380	338	-2	7	3	186	208
-4	-6	3	104	101	-2	-3	3	420	479	1	0	3	627	770	4	3	3	509	441	-1	7	3	197	218
-3	-6	3	203	214	-1	-3	3	564	624	2	0	3	588	624	5	3	3	413	378	0	7	3	312	324
-2	-6	3	290	294	0	-3	3	424	489	3	0	3	724	772	6	3	3	209	190	1	7	3	390	393
-1	-6	3	238	234	1	-3	3	408	510	4	0	3	459	614	7	3	3	129	122	2	7	3	335	340
0	-6	3	225	228	2	-3	3	630	635	5	0	3	307	299	8	3	3	102	108	3	7	3	233	229
1	-6	3	285	274	3	-3	3	594	593	6	0	3	265	243	-5	4	3	167	185	4	7	3	234	226
2	-6	3	419	403	4	-3	3	465	449	7	0	3	221	204	-4	4	3	233	251	5	7	3	214	204
3	-6	3	335	337	5	-3	3	312	291	8	0	3	142	121	-3	4	3	203	198	6	7	3	150	154
4	-6	3	209	199	6	-3	3	239	210	-6	1	3	109	120	-2	4	3	214	206	7	7	3	103	101
5	-6	3	181	177	7	-3	3	202	185	-5	1	3	213	212	-1	4	3	403	381	-2	8	3	119	140
6	-6	3	180	173	8	-3	3	131	123	-4	1	3	254	252	0	4	3	541	510	-1	8	3	108	124
7	-6	3	143	131	-6	-2	3	136	150	-3	1	3	179	162	1	4	3	591	528	0	8	3	137	159
-7	-5	3	72	73	-5	-2	3	193	199	-2	1	3	214	204	2	4	3	434	422	1	8	3	188	200
-6	-5	3	123	136	-4	-2	3	196	199	-1	1	3	629	571	3	4	3	311	286	2	8	3	180	182
-5	-5	3	135	148	-3	-2	3	155	162	0	1	3	645	625	4	4	3	438	387	3	8	3	158	165
-4	-5	3	140	148	-2	-2	3	305	321	1	1	3	437	396	5	4	3	380	339	4	8	3	117	134
-3	-5	3	203	222	-1	-2	3	581	615	2	1	3	280	293	6	4	3	225	216	5	8	3	116	124

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(3-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
6	8	3	87	114	3	-7	4	354	349	-6	-3	4	85	95	-4	0	4	314	316	-1	3	4	451	418
-1	9	3	122	154	4	-7	4	273	269	-5	-3	4	199	199	-3	0	4	375	366	0	3	4	474	428
0	9	3	115	130	5	-7	4	170	174	-4	-3	4	174	183	-2	0	4	320	314	1	3	4	780	735
1	9	3	148	174	6	-7	4	157	155	-3	-3	4	171	183	-1	0	4	461	439	2	3	4	567	555
2	9	3	180	209	7	-7	4	121	97	-2	-3	4	290	297	1	0	4	780	852	3	3	4	415	386
3	9	3	95	100	-5	-6	4	102	107	-1	-3	4	450	478	2	0	4	537	559	4	3	4	453	403
4	9	3	77	89	-4	-6	4	114	114	0	-3	4	546	620	3	0	4	450	455	5	3	4	348	299
5	9	3	103	107	-3	-6	4	122	122	1	-3	4	403	494	4	0	4	417	526	6	3	4	251	225
-1	-11	4	137	140	-2	-6	4	181	177	2	-3	4	363	397	5	0	4	407	454	7	3	4	176	163
0	-11	4	123	124	-1	-6	4	320	326	3	-3	4	392	439	6	0	4	234	273	8	3	4	102	91
1	-11	4	119	128	0	-6	4	281	285	4	-3	4	510	513	7	0	4	166	145	-5	4	4	107	83
-2	-10	4	142	144	1	-6	4	195	183	5	-3	4	362	357	8	0	4	127	114	-4	4	4	143	152
-1	-10	4	147	153	2	-6	4	233	243	6	-3	4	209	198	9	0	4	90	90	-3	4	4	263	274
0	-10	4	129	138	3	-6	4	310	308	7	-3	4	155	142	-6	1	4	80	76	-2	4	4	305	307
1	-10	4	157	158	4	-6	4	314	297	8	-3	4	132	120	-5	1	4	102	112	-1	4	4	233	230
2	-10	4	158	167	5	-6	4	179	186	9	-3	4	95	83	-4	1	4	238	240	0	4	4	266	251
3	-10	4	164	174	6	-6	4	137	123	-6	-2	4	69	87	-3	1	4	300	297	1	4	4	524	488
4	-10	4	114	136	7	-6	4	133	116	-5	-2	4	166	173	-2	1	4	259	243	2	4	4	463	476
-3	-9	4	78	83	-6	-5	4	94	94	-4	-2	4	255	258	-1	1	4	222	209	3	4	4	348	328
-2	-9	4	122	124	-5	-5	4	127	135	-3	-2	4	182	188	0	1	4	398	363	4	4	4	341	303
-1	-9	4	158	159	-4	-5	4	188	197	-2	-2	4	221	216	1	1	4	660	610	5	4	4	287	260
0	-9	4	92	96	-3	-5	4	197	207	-1	-2	4	363	370	2	1	4	443	465	6	4	4	224	204
1	-9	4	110	92	-2	-5	4	208	211	0	-2	4	392	417	3	1	4	321	302	7	4	4	162	154
2	-9	4	143	146	-1	-5	4	338	349	1	-2	4	356	424	4	1	4	287	286	8	4	4	104	109
3	-9	4	146	150	0	-5	4	372	380	2	-2	4	240	273	5	1	4	344	334	-4	5	4	104	130
4	-9	4	110	123	1	-5	4	204	230	3	-2	4	205	245	6	1	4	277	272	-3	5	4	203	221
5	-9	4	95	92	2	-5	4	273	254	4	-2	4	341	383	7	1	4	160	150	-2	5	4	266	277
-5	-8	4	108	107	3	-5	4	252	259	5	-2	4	285	290	8	1	4	98	99	-1	5	4	182	186
-4	-8	4	116	107	4	-5	4	242	230	6	-2	4	122	125	9	1	4	88	82	0	5	4	142	133
-3	-8	4	139	136	5	-5	4	197	206	7	-2	4	177	161	-5	2	4	123	129	1	5	4	332	319
-2	-8	4	236	238	6	-5	4	119	123	8	-2	4	145	127	-4	2	4	344	348	2	5	4	359	353
-1	-8	4	279	269	7	-5	4	104	90	-6	-1	4	116	126	-3	2	4	353	349	3	5	4	187	184
0	-8	4	191	182	8	-5	4	86	83	-5	-1	4	202	206	-2	2	4	225	199	4	5	4	207	193
1	-8	4	183	181	-6	-4	4	81	85	-4	-1	4	320	322	-1	2	4	379	356	5	5	4	143	135
2	-8	4	227	228	-5	-4	4	195	206	-3	-1	4	357	363	0	2	4	443	417	6	5	4	161	152
3	-8	4	203	202	-4	-4	4	324	334	-2	-1	4	410	393	1	2	4	643	589	7	5	4	164	160
4	-8	4	183	180	-3	-4	4	154	168	-1	-1	4	451	452	2	2	4	506	513	-4	6	4	125	154
5	-8	4	83	87	-2	-4	4	293	309	0	-1	4	604	612	3	2	4	113	100	-3	6	4	230	255
6	-8	4	74	70	-1	-4	4	632	680	1	-1	4	803	920	4	2	4	316	287	-2	6	4	286	317
-6	-7	4	89	85	0	-4	4	553	581	2	-1	4	404	431	5	2	4	358	336	-1	6	4	243	251
-5	-7	4	95	107	1	-4	4	515	588	3	-1	4	235	273	6	2	4	201	183	0	6	4	274	276
-4	-7	4	131	130	2	-4	4	361	373	4	-1	4	330	450	7	2	4	137	121	1	6	4	397	390
-3	-7	4	159	170	3	-4	4	352	364	5	-1	4	248	275	8	2	4	110	96	2	6	4	326	321
-2	-7	4	281	285	4	-4	4	495	491	6	-1	4	259	262	-6	3	4	74	86	3	6	4	286	280
-1	-7	4	330	329	5	-4	4	305	301	7	-1	4	170	164	-5	3	4	162	181	4	6	4	213	207
0	-7	4	335	335	6	-4	4	155	147	9	-1	4	102	75	-4	3	4	230	246	5	6	4	161	161
1	-7	4	345	340	7	-4	4	136	127	-6	0	4	80	86	-3	3	4	281	278	6	6	4	171	170
2	-7	4	294	286	8	-4	4	111	108	-5	0	4	155	161	-2	3	4	499	490	7	6	4	108	96

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(3-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-3	7	4	136	164	1	-8	5	260	249	-4	-4	5	189	193	1	-1	5	606	630	6	2	5	198	178
-2	7	4	215	245	2	-8	5	134	136	-3	-4	5	286	288	2	-1	5	451	488	7	2	5	198	191
-1	7	4	231	255	3	-8	5	158	152	-2	-4	5	411	426	3	-1	5	462	502	-5	3	5	118	124
0	7	4	190	203	4	-8	5	200	195	-1	-4	5	247	271	4	-1	5	227	301	-4	3	5	102	126
1	7	4	261	275	5	-8	5	122	130	0	-4	5	414	417	5	-1	5	218	247	-3	3	5	291	309
2	7	4	318	328	6	-8	5	98	98	1	-4	5	617	695	6	-1	5	228	255	-2	3	5	438	440
3	7	4	277	285	-5	-7	5	104	96	2	-4	5	432	447	7	-1	5	125	134	-1	3	5	336	325
4	7	4	218	222	-4	-7	5	159	151	3	-4	5	330	368	8	-1	5	116	108	0	3	5	423	394
5	7	4	149	153	-3	-7	5	161	152	4	-4	5	310	317	9	-1	5	98	83	1	3	5	526	497
6	7	4	142	144	-2	-7	5	173	169	5	-4	5	275	267	-5	0	5	119	120	2	3	5	528	504
7	7	4	105	108	-1	-7	5	250	255	6	-4	5	239	234	-4	0	5	173	182	3	3	5	503	498
-1	8	4	120	139	0	-7	5	387	371	7	-4	5	140	140	-3	0	5	325	327	4	3	5	374	345
0	8	4	116	124	1	-7	5	328	315	-5	-3	5	78	89	-2	0	5	437	427	5	3	5	239	219
1	8	4	129	144	2	-7	5	262	260	-4	-3	5	186	193	-1	0	5	390	370	6	3	5	258	232
2	8	4	189	200	3	-7	5	275	274	-3	-3	5	293	298	1	0	5	654	628	7	3	5	188	174
3	8	4	139	155	4	-7	5	256	251	-2	-3	5	214	222	2	0	5	741	753	8	3	5	107	100
4	8	4	118	121	5	-7	5	216	218	-1	-3	5	198	207	3	0	5	507	514	-4	4	5	88	92
5	8	4	112	127	6	-7	5	142	133	0	-3	5	374	391	4	0	5	292	351	-3	4	5	128	143
6	8	4	77	97	7	-7	5	88	89	1	-3	5	528	613	5	0	5	292	313	-2	4	5	275	289
1	9	4	134	155	-5	-6	5	87	89	2	-3	5	456	499	6	0	5	282	304	-1	4	5	296	296
2	9	4	131	152	-4	-6	5	150	150	3	-3	5	278	313	7	0	5	177	207	0	4	5	247	239
3	9	4	116	125	-3	-6	5	127	133	4	-3	5	284	316	8	0	5	98	111	1	4	5	305	296
4	9	4	117	139	-2	-6	5	105	102	5	-3	5	314	328	-6	1	5	90	93	2	4	5	334	339
0	-11	5	107	114	-1	-6	5	175	179	6	-3	5	269	263	-5	1	5	89	99	3	4	5	386	379
1	-11	5	128	125	0	-6	5	282	275	7	-3	5	182	170	-4	1	5	135	141	4	4	5	319	303
-3	-10	5	81	78	1	-6	5	332	320	8	-3	5	99	100	-3	1	5	212	211	5	4	5	218	204
-2	-10	5	118	102	2	-6	5	194	201	-6	-2	5	88	87	-2	1	5	313	302	6	4	5	196	190
-1	-10	5	104	118	3	-6	5	172	173	-5	-2	5	80	99	-1	1	5	308	293	7	4	5	174	166
0	-10	5	159	156	4	-6	5	226	228	-4	-2	5	169	169	0	1	5	245	230	-4	5	5	100	108
1	-10	5	136	136	5	-6	5	231	228	-3	-2	5	282	293	1	1	5	354	334	-3	5	5	129	156
2	-10	5	134	136	6	-6	5	152	158	-2	-2	5	286	283	2	1	5	456	453	-2	5	5	203	223
3	-10	5	146	150	7	-6	5	89	93	-1	-2	5	130	146	3	1	5	377	364	-1	5	5	243	256
4	-10	5	120	134	-6	-5	5	72	66	0	-2	5	276	268	4	1	5	254	286	0	5	5	213	214
-4	-9	5	72	78	-5	-5	5	125	125	1	-2	5	514	534	5	1	5	269	270	1	5	5	209	202
-3	-9	5	68	67	-4	-5	5	197	200	2	-2	5	335	375	6	1	5	209	203	2	5	5	182	179
-2	-9	5	93	86	-3	-5	5	165	169	3	-2	5	142	173	7	1	5	181	168	3	5	5	277	267
-1	-9	5	118	121	-2	-5	5	182	179	4	-2	5	200	259	8	1	5	116	123	4	5	5	255	252
0	-9	5	133	130	-1	-5	5	311	311	5	-2	5	223	247	-5	2	5	131	133	5	5	5	114	115
1	-9	5	141	133	0	-5	5	309	304	6	-2	5	233	233	-4	2	5	132	136	6	5	5	144	138
2	-9	5	89	94	1	-5	5	287	330	7	-2	5	158	155	-3	2	5	221	211	7	5	5	107	102
3	-9	5	98	102	2	-5	5	259	274	9	-2	5	104	76	-2	2	5	534	520	8	5	5	87	70
4	-9	5	119	130	3	-5	5	130	139	-6	-1	5	91	89	-1	2	5	414	401	-3	6	5	122	136
5	-9	5	107	102	4	-5	5	260	253	-5	-1	5	107	108	0	2	5	120	100	-2	6	5	223	255
-4	-8	5	125	122	5	-5	5	211	221	-4	-1	5	256	261	1	2	5	479	429	-1	6	5	301	329
-3	-8	5	153	145	6	-5	5	130	116	-3	-1	5	378	375	2	2	5	468	472	0	6	5	266	289
-2	-8	5	155	144	7	-5	5	101	103	-2	-1	5	438	417	3	2	5	407	374	1	6	5	226	233
-1	-8	5	206	200	-6	-4	5	77	71	-1	-1	5	350	361	4	2	5	305	311	2	6	5	275	277
0	-8	5	280	267	-5	-4	5	123	137	0	-1	5	510	471	5	2	5	134	122	3	6	5	320	321

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [Ni(3-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
4	6	5	237	228	0	-7	6	235	224	-3	-3	6	174	180	4	0	6	394	443	1	4	6	253	249
5	6	5	142	149	1	-7	6	332	307	-2	-3	6	313	311	5	0	6	245	265	2	4	6	194	193
6	6	5	131	126	2	-7	6	329	324	-1	-3	6	292	295	6	0	6	206	207	3	4	6	305	306
7	6	5	114	103	3	-7	6	212	216	0	-3	6	220	209	7	0	6	178	183	4	4	6	324	312
-2	7	5	138	175	4	-7	6	199	190	1	-3	6	299	319	8	0	6	131	138	5	4	6	213	205
-1	7	5	195	231	5	-7	6	184	198	2	-3	6	389	421	-5	1	6	114	115	6	4	6	167	160
0	7	5	227	244	6	-7	6	157	152	3	-3	6	396	448	-4	1	6	88	101	7	4	6	128	128
1	7	5	223	236	7	-7	6	98	102	4	-3	6	260	308	-3	1	6	114	123	8	4	6	106	95
2	7	5	195	211	-4	-6	6	82	86	5	-3	6	201	217	-2	1	6	286	282	-2	5	6	136	139
3	7	5	241	251	-3	-6	6	140	141	6	-3	6	220	209	-1	1	6	328	313	-1	5	6	215	234
4	7	5	226	230	-2	-6	6	194	188	7	-3	6	181	178	0	1	6	197	186	0	5	6	243	257
5	7	5	163	169	-1	-6	6	146	137	8	-3	6	103	106	1	1	6	278	256	1	5	6	203	208
6	7	5	128	126	0	-6	6	129	116	-5	-2	6	102	99	2	1	6	329	332	2	5	6	155	155
0	8	5	104	124	1	-6	6	238	231	-4	-2	6	112	125	3	1	6	348	332	3	5	6	228	219
1	8	5	107	119	2	-6	6	265	284	-3	-2	6	188	186	4	1	6	299	333	4	5	6	183	183
2	8	5	110	133	3	-6	6	201	216	-2	-2	6	288	274	5	1	6	174	185	5	5	6	160	157
3	8	5	118	137	4	-6	6	145	150	-1	-2	6	325	311	6	1	6	169	171	6	5	6	142	142
4	8	5	151	170	5	-6	6	158	162	0	-2	6	223	211	7	1	6	188	189	7	5	6	77	85
5	8	5	101	103	6	-6	6	158	147	1	-2	6	179	193	8	1	6	106	105	8	5	6	91	79
-1	-10	6	109	95	7	-6	6	126	118	2	-2	6	305	328	-4	2	6	149	149	-2	6	6	147	179
0	-10	6	137	133	8	-6	6	93	77	3	-2	6	405	425	-3	2	6	164	173	-1	6	6	188	214
1	-10	6	148	141	-4	-5	6	119	119	4	-2	6	182	246	-2	2	6	274	275	0	6	6	273	300
2	-10	6	122	128	-3	-5	6	217	214	5	-2	6	86	109	-1	2	6	275	282	1	6	6	279	300
3	-10	6	86	104	-2	-5	6	301	295	6	-2	6	177	192	0	2	6	499	467	2	6	6	206	211
4	-10	6	120	117	-1	-5	6	146	150	7	-2	6	153	160	1	2	6	392	378	3	6	6	205	205
-3	-9	6	102	87	0	-5	6	145	132	8	-2	6	106	106	2	2	6	140	127	4	6	6	229	233
-2	-9	6	93	80	1	-5	6	395	403	-5	-1	6	157	154	3	2	6	412	381	5	6	6	191	189
-1	-9	6	87	70	2	-5	6	317	315	-4	-1	6	125	134	4	2	6	333	344	6	6	6	122	125
0	-9	6	128	121	3	-5	6	193	198	-3	-1	6	192	188	5	2	6	191	184	7	6	6	82	84
1	-9	6	139	139	4	-5	6	169	175	-2	-1	6	440	438	6	2	6	174	180	0	7	6	185	215
2	-9	6	97	99	5	-5	6	115	128	-1	-1	6	476	465	7	2	6	133	117	1	7	6	194	227
4	-9	6	99	102	6	-5	6	179	174	0	-1	6	387	350	-4	3	6	126	141	2	7	6	182	198
5	-9	6	92	91	7	-5	6	122	128	1	-1	6	359	358	-3	3	6	154	161	3	7	6	176	196
-4	-8	6	119	111	-5	-4	6	98	101	2	-1	6	519	510	-2	3	6	227	234	4	7	6	175	189
-3	-8	6	132	131	-4	-4	6	121	124	3	-1	6	494	512	-1	3	6	436	429	5	7	6	163	162
-2	-8	6	152	147	-3	-4	6	269	267	4	-1	6	217	281	0	3	6	478	472	6	7	6	115	118
-1	-8	6	175	163	-2	-4	6	299	310	5	-1	6	213	239	1	3	6	329	306	2	8	6	83	92
0	-8	6	200	189	-1	-4	6	282	285	6	-1	6	192	209	2	3	6	325	313	3	8	6	77	97
1	-8	6	243	230	0	-4	6	442	418	7	-1	6	151	160	3	3	6	448	442	-1	-10	7	101	80
2	-8	6	206	203	1	-4	6	363	405	8	-1	6	105	112	4	3	6	416	390	0	-10	7	80	72
3	-8	6	174	174	2	-4	6	431	439	-5	0	6	110	120	5	3	6	271	253	1	-10	7	128	115
4	-8	6	110	115	3	-4	6	413	436	-4	0	6	99	104	6	3	6	194	180	2	-10	7	146	130
5	-8	6	134	119	4	-4	6	249	271	-3	0	6	178	174	7	3	6	141	135	3	-10	7	120	115
6	-8	6	119	116	5	-4	6	227	237	-2	0	6	360	354	8	3	6	116	108	-2	-9	7	91	92
-4	-7	6	98	89	6	-4	6	221	213	-1	0	6	469	454	-3	4	6	116	123	-1	-9	7	107	92
-3	-7	6	161	160	7	-4	6	148	140	1	0	6	372	344	-2	4	6	124	138	0	-9	7	87	73
-2	-7	6	209	187	8	-4	6	86	93	2	0	6	433	436	-1	4	6	226	233	1	-9	7	88	86
-1	-7	6	188	180	-4	-3	6	89	95	3	0	6	576	563	0	4	6	317	334	2	-9	7	137	131

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(3-picNO)2][AuCl4]

H	K	L	10Fo	10Fc
3	-9	7	119	113
-3	-8	7	118	106
-2	-8	7	187	174
-1	-8	7	161	148
0	-8	7	146	138
1	-8	7	188	174
2	-8	7	218	201
3	-8	7	181	180
4	-8	7	122	121
5	-8	7	115	113
6	-8	7	89	89
-3	-7	7	134	115
-2	-7	7	170	161
-1	-7	7	197	189
0	-7	7	186	168
1	-7	7	221	204
2	-7	7	269	257
3	-7	7	270	254
4	-7	7	193	197
5	-7	7	129	136
6	-7	7	131	126
7	-7	7	109	111
-3	-6	7	96	84
-2	-6	7	153	147
-1	-6	7	155	159
0	-6	7	157	147
1	-6	7	179	163
2	-6	7	176	175
3	-6	7	191	193
4	-6	7	199	198
5	-6	7	106	134
6	-6	7	122	114
7	-6	7	119	110
8	-6	7	87	69
-4	-5	7	80	81
-3	-5	7	126	115
-2	-5	7	217	209
-1	-5	7	263	255
0	-5	7	305	281
1	-5	7	131	147
2	-5	7	144	135
3	-5	7	362	352
4	-5	7	209	221
5	-5	7	99	106
6	-5	7	119	120
7	-5	7	105	97
-5	-4	7	95	89
-4	-4	7	107	105
-3	-4	7	149	152
-2	-4	7	231	230
-1	-4	7	391	371
0	-4	7	324	314
1	-4	7	225	240
2	-4	7	391	381
3	-4	7	389	396
4	-4	7	282	305
5	-4	7	200	210
6	-4	7	163	154
7	-4	7	140	144
8	-4	7	115	106
-5	-3	7	102	100
-4	-3	7	108	105
-3	-3	7	100	85
-2	-3	7	165	164
-1	-3	7	287	288
0	-3	7	332	318
1	-3	7	206	221
2	-3	7	239	235
3	-3	7	350	364
4	-3	7	257	311
5	-3	7	185	217
6	-3	7	176	182
7	-3	7	146	147
8	-3	7	97	103
9	-3	7	97	73
-5	-2	7	119	111
-4	-2	7	109	117
-3	-2	7	93	94
-2	-2	7	200	203
-1	-2	7	306	303
0	-2	7	306	271
1	-2	7	224	221
2	-2	7	187	190
3	-2	7	260	264
4	-2	7	206	257
5	-2	7	192	227
6	-2	7	134	152
7	-2	7	88	94
8	-2	7	103	104
-5	-1	7	137	127
-4	-1	7	149	151
-3	-1	7	199	193
-2	-1	7	218	223
-1	-1	7	337	321
0	-1	7	504	474
1	-1	7	378	379
2	-1	7	293	280
3	-1	7	355	349
4	-1	7	333	386
5	-1	7	238	268
6	-1	7	141	148
7	-1	7	127	135
8	-1	7	107	115
9	-1	7	83	73
-4	0	7	150	158
-3	0	7	145	142
-2	0	7	157	155
-1	0	7	286	279
1	0	7	432	417
2	0	7	303	298
3	0	7	340	326
4	0	7	344	364
5	0	7	308	325
6	0	7	209	213
7	0	7	143	150
8	0	7	104	107
-4	1	7	131	141
-3	1	7	114	122
-2	1	7	96	108
-1	1	7	185	186
0	1	7	401	380
1	1	7	329	317
2	1	7	73	77
3	1	7	258	238
4	1	7	301	352
5	1	7	212	210
6	1	7	175	174
7	1	7	110	115
8	1	7	92	91
9	1	7	89	90
-4	2	7	122	145
-3	2	7	197	199
-2	2	7	161	168
-1	2	7	248	240
0	2	7	413	394
1	2	7	226	259
2	2	7	294	277
3	2	7	335	326
4	2	7	183	192
5	2	7	237	225
6	2	7	172	182
7	2	7	98	102
8	2	7	110	98
-3	3	7	175	187
-2	3	7	149	158
-1	3	7	217	214
0	3	7	355	357
1	3	7	431	420
2	3	7	336	331
3	3	7	281	271
4	3	7	282	266
5	3	7	284	271
6	3	7	206	206
7	3	7	129	127
8	3	7	103	89
-2	4	7	117	124
-1	4	7	146	156
0	4	7	206	216
1	4	7	261	263
2	4	7	245	253
3	4	7	199	201
4	4	7	185	186
5	4	7	219	215
6	4	7	194	191
7	4	7	99	103
8	4	7	89	79
-2	5	7	153	163
-1	5	7	88	91
0	5	7	171	184
1	5	7	251	266
2	5	7	189	194
3	5	7	143	147
4	5	7	142	146
5	5	7	175	172
6	5	7	111	122
7	5	7	80	83
0	6	7	192	221
1	6	7	239	260
2	6	7	227	240
3	6	7	194	211
4	6	7	155	159
5	6	7	153	149
6	6	7	137	140
2	7	7	160	181
3	7	7	131	160
4	7	7	153	160
1-10		8	87	75
2-10		8	100	86
3-10		8	107	109
-1	-9	8	92	91
0	-9	8	92	83
1	-9	8	106	82
2	-9	8	89	79
3	-9	8	101	93
4	-9	8	90	98
5	-9	8	84	74
-2	-8	8	111	96
-1	-8	8	167	148
0	-8	8	209	184
1	-8	8	152	129
2	-8	8	142	128
3	-8	8	175	160
4	-8	8	162	150
5	-8	8	119	103
-2	-7	8	110	100
-1	-7	8	196	173
0	-7	8	224	194
1	-7	8	188	167
2	-7	8	153	144
3	-7	8	215	197
4	-7	8	230	208
5	-7	8	144	151
6	-7	8	107	101
7	-7	8	101	83
-3	-6	8	80	69
-2	-6	8	83	87
-1	-6	8	147	139
0	-6	8	204	177
1	-6	8	128	124
2	-6	8	98	100
3	-6	8	203	192
4	-6	8	186	182
5	-6	8	86	107
6	-6	8	118	111
7	-6	8	80	88
-4	-5	8	118	103
-3	-5	8	131	123
-2	-5	8	96	106
-1	-5	8	203	176
0	-5	8	284	262
1	-5	8	199	199
2	-5	8	231	207
3	-5	8	178	174
4	-5	8	143	137
5	-5	8	182	200
6	-5	8	129	126
7	-5	8	92	72
8	-5	8	94	72
-4	-4	8	132	125
-3	-4	8	118	117

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(3-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-2	-4	8	126	129	7	-1	8	104	123	3	4	8	197	199	3	-5	9	124	125	7	-1	9	134	141
-1	-4	8	247	231	-3	0	8	161	169	4	4	8	157	168	4	-5	9	155	156	-2	0	9	162	171
0	-4	8	340	319	-2	0	8	163	171	5	4	8	159	158	5	-5	9	132	153	-1	0	9	173	170
1	-4	8	344	337	-1	0	8	167	157	6	4	8	137	138	6	-5	9	106	95	1	0	9	211	206
2	-4	8	234	232	1	0	8	353	343	7	4	8	110	112	7	-5	9	92	91	2	0	9	322	301
3	-4	8	218	224	2	0	8	327	320	0	5	8	142	162	-3	-4	9	134	128	3	0	9	290	282
4	-4	8	280	294	3	0	8	307	295	1	5	8	116	130	-2	-4	9	159	152	4	0	9	161	173
5	-4	8	236	248	4	0	8	263	269	2	5	8	172	184	-1	-4	9	126	121	5	0	9	180	186
6	-4	8	155	158	5	0	8	230	233	3	5	8	194	208	0	-4	9	193	175	6	0	9	209	209
7	-4	8	110	107	6	0	8	209	204	4	5	8	122	127	1	-4	9	295	282	7	0	9	125	124
8	-4	8	92	81	7	0	8	152	154	5	5	8	95	106	2	-4	9	302	284	8	0	9	98	83
-4	-3	8	110	105	8	0	8	89	96	6	5	8	111	117	3	-4	9	228	223	-2	1	9	123	144
-3	-3	8	122	125	-3	1	8	170	175	2	6	8	193	210	4	-4	9	166	167	-1	1	9	188	184
-2	-3	8	104	109	-2	1	8	149	158	3	6	8	190	215	5	-4	9	161	180	0	1	9	134	141
-1	-3	8	151	141	-1	1	8	92	96	4	6	8	148	155	6	-4	9	172	171	1	1	9	95	110
0	-3	8	260	239	0	1	8	182	172	5	6	8	127	131	7	-4	9	115	115	2	1	9	236	223
1	-3	8	291	287	1	1	8	242	242	0	-9	9	119	95	-3	-3	9	102	105	3	1	9	209	210
2	-3	8	240	236	2	1	8	308	304	1	-9	9	97	85	-2	-3	9	124	129	4	1	9	156	170
3	-3	8	182	187	3	1	8	257	257	4	-9	9	86	80	-1	-3	9	111	108	5	1	9	188	188
4	-3	8	212	235	4	1	8	63	77	-1	-8	9	128	104	0	-3	9	145	138	6	1	9	95	96
5	-3	8	245	254	5	1	8	193	181	0	-8	9	149	130	1	-3	9	231	220	7	1	9	101	100
6	-3	8	158	171	6	1	8	233	235	1	-8	9	154	143	2	-3	9	234	222	8	1	9	110	110
7	-3	8	92	101	7	1	8	109	111	2	-8	9	161	139	3	-3	9	194	194	-1	2	9	212	220
8	-3	8	102	97	-3	2	8	162	183	3	-8	9	123	108	4	-3	9	154	173	0	2	9	138	149
-4	-2	8	116	129	-2	2	8	158	173	4	-8	9	124	114	5	-3	9	161	160	1	2	9	163	173
-3	-2	8	157	152	-1	2	8	191	187	5	-8	9	128	109	6	-3	9	155	158	2	2	9	251	247
-2	-2	8	122	120	0	2	8	211	214	-2	-7	9	92	77	7	-3	9	119	129	3	2	9	263	259
-1	-2	8	105	105	1	2	8	258	298	-1	-7	9	74	79	-3	-2	9	137	146	4	2	9	191	205
0	-2	8	312	290	2	2	8	352	345	0	-7	9	158	142	-2	-2	9	166	170	5	2	9	132	122
1	-2	8	314	325	3	2	8	189	179	1	-7	9	202	183	-1	-2	9	140	137	6	2	9	114	119
2	-2	8	178	170	4	2	8	161	167	2	-7	9	177	157	0	-2	9	143	136	7	2	9	134	130
3	-2	8	169	167	5	2	8	238	234	3	-7	9	161	136	1	-2	9	160	156	-1	3	9	185	193
4	-2	8	182	201	6	2	8	163	159	4	-7	9	144	129	2	-2	9	294	272	0	3	9	189	197
5	-2	8	196	210	7	2	8	114	108	5	-7	9	136	133	3	-2	9	223	233	1	3	9	184	186
6	-2	8	130	143	-2	3	8	190	214	6	-7	9	137	120	4	-2	9	101	112	2	3	9	216	218
7	-2	8	88	113	-1	3	8	179	191	0	-6	9	157	131	5	-2	9	143	138	3	3	9	241	241
8	-2	8	80	90	0	3	8	185	189	1	-6	9	179	163	6	-2	9	156	156	4	3	9	233	227
-4	-1	8	119	129	1	3	8	266	269	2	-6	9	158	141	7	-2	9	113	114	5	3	9	176	173
-3	-1	8	197	195	2	3	8	346	346	3	-6	9	94	97	-3	-1	9	136	145	6	3	9	128	128
-2	-1	8	160	161	3	3	8	294	296	4	-6	9	84	87	-2	-1	9	197	196	7	3	9	110	118
-1	-1	8	236	221	4	3	8	205	202	5	-6	9	150	157	-1	-1	9	206	196	0	4	9	147	156
0	-1	8	359	339	5	3	8	226	204	6	-6	9	125	123	0	-1	9	164	162	1	4	9	79	92
1	-1	8	393	373	6	3	8	187	181	-3	-5	9	115	111	1	-1	9	266	259	2	4	9	138	133
2	-1	8	336	331	7	3	8	125	127	-2	-5	9	111	111	2	-1	9	362	345	3	4	9	215	224
3	-1	8	253	252	-1	4	8	101	110	-1	-5	9	158	133	3	-1	9	304	284	4	4	9	159	166
4	-1	8	221	243	0	4	8	109	121	0	-5	9	169	154	4	-1	9	174	189	5	4	9	116	118
5	-1	8	251	257	1	4	8	207	217	1	-5	9	222	207	5	-1	9	171	167	6	4	9	113	115
6	-1	8	200	205	2	4	8	215	229	2	-5	9	238	212	6	-1	9	173	169	2	5	9	143	154

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(3-picNO)2][AuCl4]

H	K	L	10Fo	10Fc
3	5	9	138	155
4	5	9	133	131
5	5	9	116	123
1	-8	10	157	125
2	-8	10	154	125
3	-8	10	112	100
4	-8	10	98	90
0	-7	10	97	87
1	-7	10	125	109
2	-7	10	164	144
3	-7	10	145	135
4	-7	10	102	104
5	-7	10	110	105
6	-7	10	113	94
-1	-6	10	104	88
1	-6	10	95	84
2	-6	10	170	148
3	-6	10	144	129
4	-6	10	92	92
5	-6	10	93	86
6	-6	10	69	71
-1	-5	10	131	124
0	-5	10	101	96
1	-5	10	170	146
2	-5	10	203	177
3	-5	10	173	162
4	-5	10	137	126
5	-5	10	93	89
6	-5	10	116	110
7	-5	10	111	93
-2	-4	10	139	132
-1	-4	10	176	155
0	-4	10	155	137
1	-4	10	137	136
2	-4	10	221	202
3	-4	10	247	233
4	-4	10	184	180
5	-4	10	115	132
6	-4	10	123	117
7	-4	10	119	107
-2	-3	10	122	118
-1	-3	10	126	123
0	-3	10	114	109
1	-3	10	98	102
2	-3	10	187	176
3	-3	10	233	222
4	-3	10	128	138
5	-3	10	119	116
6	-3	10	129	128
7	-3	10	104	104
-2	-2	10	97	93
-1	-2	10	197	182
0	-2	10	150	148
1	-2	10	119	115
2	-2	10	188	173
3	-2	10	173	168
4	-2	10	173	167
5	-2	10	124	137
6	-2	10	104	95
7	-2	10	92	94
-1	-1	10	220	204
0	-1	10	205	196
1	-1	10	168	161
2	-1	10	192	181
3	-1	10	248	244
4	-1	10	214	227
5	-1	10	168	165
6	-1	10	125	123
7	-1	10	93	99
-1	0	10	182	176
1	0	10	122	127
2	0	10	166	164
3	0	10	230	224
4	0	10	218	221
5	0	10	177	174
6	0	10	98	100
7	0	10	111	103
8	0	10	108	114
-1	1	10	161	149
0	1	10	132	148
1	1	10	142	134
2	1	10	149	142
3	1	10	132	143
4	1	10	172	179
5	1	10	135	131
6	1	10	79	97
7	1	10	109	117
0	2	10	206	211
1	2	10	158	178
2	2	10	121	128
3	2	10	179	168
4	2	10	199	199
5	2	10	158	160
6	2	10	111	108
7	2	10	84	81
1	3	10	161	166
2	3	10	151	156
3	3	10	180	185
4	3	10	177	184
5	3	10	165	147
6	3	10	131	124
4	4	10	108	117
2	-7	11	119	101
3	-7	11	137	112
4	-7	11	120	99
1	-6	11	79	73
3	-6	11	94	93
4	-6	11	119	110
5	-6	11	89	79
0	-5	11	140	125
1	-5	11	114	101
2	-5	11	110	95
3	-5	11	175	144
4	-5	11	143	136
5	-5	11	90	94
6	-5	11	69	73
0	-4	11	161	148
1	-4	11	140	133
2	-4	11	140	123
3	-4	11	164	147
4	-4	11	160	156
5	-4	11	138	134
6	-4	11	115	104
7	-4	11	97	78
0	-3	11	164	150
1	-3	11	101	94
2	-3	11	95	93
3	-3	11	108	117
4	-3	11	164	152
5	-3	11	155	148
6	-3	11	87	80
0	-2	11	127	124
1	-2	11	149	146
2	-2	11	115	111
3	-2	11	131	117
4	-2	11	164	160
5	-2	11	119	118
6	-2	11	90	86
7	-2	11	90	79
0	-1	11	197	176
1	-1	11	185	184
2	-1	11	167	152
3	-1	11	143	146
4	-1	11	161	162
5	-1	11	159	159
6	-1	11	122	116
7	-1	11	88	86
1	0	11	181	174
2	0	11	149	141
3	0	11	95	107
4	0	11	155	151
5	0	11	168	165
6	0	11	112	118
7	0	11	106	95
1	1	11	149	157
2	1	11	106	108
3	1	11	93	100
4	1	11	133	138
5	1	11	121	123
6	1	11	106	103
3	2	11	127	128
4	2	11	113	115
5	2	11	116	127
3	-5	12	94	80
4	-5	12	111	91
2	-4	12	131	113
3	-4	12	122	105
4	-4	12	132	109
5	-4	12	128	115
2	-3	12	140	128
4	-3	12	94	89
5	-3	12	108	101
2	-2	12	110	109
3	-2	12	106	93
4	-2	12	101	91
5	-2	12	102	103
3	-1	12	132	120
4	-1	12	120	113
5	-1	12	131	121

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(4-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	0	0	697	635	-2	3	0	516	498	1	7	0	309	309	-5	-3	1	362	375	-4	0	1	630	620
2	0	0	1400	1238	-1	3	0	600	583	2	7	0	264	249	-4	-3	1	471	494	-3	0	1	416	422
3	0	0	949	819	0	3	0	605	602	3	7	0	236	266	-3	-3	1	637	636	-2	0	1	976	978
4	0	0	735	690	1	3	0	662	640	4	7	0	188	184	-2	-3	1	905	876	-1	0	1	885	960
5	0	0	463	413	2	3	0	673	626	0	8	0	177	179	-1	-3	1	594	614	0	0	1	670	879
6	0	0	389	377	3	3	0	398	376	1	8	0	218	195	0	-3	1	1063	1049	1	0	1	814	710
7	0	0	268	261	4	3	0	470	451	2	8	0	184	175	1	-3	1	815	792	2	0	1	1811	1237
-8	1	0	197	195	5	3	0	370	360	4	8	0	185	185	2	-3	1	737	692	3	0	1	855	562
-7	1	0	158	176	6	3	0	227	245	-3	-7	1	213	217	3	-3	1	614	567	4	0	1	687	512
-6	1	0	326	300	7	3	0	221	245	-2	-7	1	189	175	4	-3	1	426	398	5	0	1	650	505
-5	1	0	290	261	-5	4	0	174	190	-1	-7	1	241	237	5	-3	1	405	373	6	0	1	348	320
-4	1	0	410	386	-4	4	0	210	216	0	-7	1	166	175	6	-3	1	244	243	7	0	1	300	282
-3	1	0	478	410	-3	4	0	241	248	1	-7	1	182	180	7	-3	1	157	192	8	0	1	201	224
-2	1	0	678	618	-2	4	0	325	322	-5	-6	1	172	169	-8	-2	1	168	186	-7	1	1	155	185
-1	1	0	881	798	-1	4	0	292	294	-3	-6	1	262	264	-6	-2	1	243	286	-6	1	1	175	194
0	1	0	714	729	0	4	0	555	540	-2	-6	1	223	229	-5	-2	1	263	289	-5	1	1	235	224
1	1	0	1072	992	1	4	0	301	304	-1	-6	1	287	260	-4	-2	1	361	408	-4	1	1	313	308
2	1	0	1146	1075	2	4	0	576	534	0	-6	1	289	281	-3	-2	1	436	475	-3	1	1	333	314
3	1	0	667	692	3	4	0	443	419	1	-6	1	393	378	-2	-2	1	580	586	-2	1	1	518	518
4	1	0	737	782	4	4	0	490	465	3	-6	1	369	346	-1	-2	1	700	726	-1	1	1	369	366
5	1	0	546	536	5	4	0	266	242	4	-6	1	200	205	0	-2	1	850	858	0	1	1	1019	1085
6	1	0	441	453	6	4	0	399	407	5	-6	1	183	203	1	-2	1	893	865	1	1	1	683	598
7	1	0	318	346	7	4	0	163	180	-5	-5	1	232	255	2	-2	1	783	724	2	1	1	1308	927
8	1	0	197	239	-6	5	0	173	215	-4	-5	1	177	199	3	-2	1	945	822	3	1	1	877	700
9	1	0	196	209	-4	5	0	209	225	-3	-5	1	269	254	4	-2	1	663	602	4	1	1	819	769
-8	2	0	199	212	-3	5	0	191	208	-2	-5	1	234	219	5	-2	1	571	487	5	1	1	472	461
-7	2	0	263	265	-2	5	0	184	196	-1	-5	1	281	276	6	-2	1	408	383	6	1	1	519	490
-6	2	0	244	257	0	5	0	271	262	0	-5	1	198	205	7	-2	1	377	356	7	1	1	317	325
-5	2	0	406	369	1	5	0	136	130	1	-5	1	174	193	-7	-1	1	269	271	8	1	1	251	267
-4	2	0	487	454	2	5	0	180	206	2	-5	1	317	330	-6	-1	1	283	306	9	1	1	202	198
-3	2	0	284	267	3	5	0	227	205	3	-5	1	186	188	-5	-1	1	389	393	-8	2	1	187	199
-2	2	0	668	627	4	5	0	249	241	4	-5	1	237	245	-4	-1	1	385	418	-6	2	1	335	335
-1	2	0	458	434	5	5	0	202	212	5	-5	1	241	241	-3	-1	1	518	575	-5	2	1	176	185
0	2	0	478	479	6	5	0	175	202	-7	-4	1	234	248	-2	-1	1	479	539	-4	2	1	291	284
1	2	0	466	447	7	5	0	181	189	-6	-4	1	279	308	-1	-1	1	599	652	-3	2	1	220	207
2	2	0	619	565	-5	6	0	262	270	-5	-4	1	306	319	0	-1	1	580	623	-2	2	1	373	355
3	2	0	489	462	-4	6	0	281	277	-4	-4	1	537	556	1	-1	1	820	771	-1	2	1	154	-141
4	2	0	449	440	-3	6	0	239	261	-3	-4	1	385	374	2	-1	1	596	517	0	2	1	388	383
5	2	0	377	405	-2	6	0	369	369	-2	-4	1	522	512	3	-1	1	713	577	1	2	1	196	190
6	2	0	301	344	-1	6	0	296	302	-1	-4	1	556	543	4	-1	1	627	507	2	2	1	385	326
7	2	0	249	277	0	6	0	227	226	0	-4	1	363	357	5	-1	1	529	430	3	2	1	438	339
8	2	0	229	251	1	6	0	250	244	1	-4	1	390	374	6	-1	1	407	366	4	2	1	494	429
-8	3	0	163	151	2	6	0	261	264	2	-4	1	295	297	7	-1	1	306	281	5	2	1	415	388
-7	3	0	206	226	4	6	0	175	187	3	-4	1	242	243	8	-1	1	273	271	6	2	1	340	346
-6	3	0	258	256	-3	7	0	262	252	4	-4	1	212	215	9	-1	1	189	173	7	2	1	279	323
-5	3	0	350	335	-2	7	0	217	229	5	-4	1	191	183	-7	0	1	217	238	8	2	1	188	236
-4	3	0	349	356	-1	7	0	336	335	-7	-3	1	173	204	-6	0	1	290	305	9	2	1	179	213
-3	3	0	597	560	0	7	0	280	283	-6	-3	1	297	345	-5	0	1	369	362	-7	3	1	250	267

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(4-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-6	3	1	229	258	1	6	1	191	198	2	-4	2	310	301	3	-1	2	639	512	1	2	2	369	363
-5	3	1	410	392	2	6	1	286	283	3	-4	2	380	360	4	-1	2	592	475	2	2	2	612	528
-4	3	1	449	442	3	6	1	229	228	4	-4	2	285	300	5	-1	2	567	455	3	2	2	584	469
-3	3	1	419	395	4	6	1	280	261	5	-4	2	268	275	6	-1	2	462	394	4	2	2	661	458
-2	3	1	507	510	-3	7	1	253	282	6	-4	2	231	241	7	-1	2	435	367	5	2	2	476	386
-1	3	1	457	445	-2	7	1	298	305	7	-4	2	181	201	8	-1	2	254	242	6	2	2	404	371
0	3	1	443	437	-1	7	1	370	378	8	-4	2	177	172	9	-1	2	227	228	7	2	2	273	287
1	3	1	290	286	0	7	1	326	314	-6	-3	2	246	258	-7	0	2	229	254	8	2	2	192	240
2	3	1	215	202	1	7	1	377	370	-5	-3	2	228	260	-6	0	2	283	295	9	2	2	184	204
3	3	1	386	342	2	7	1	363	346	-4	-3	2	462	522	-5	0	2	335	355	-7	3	2	206	225
4	3	1	230	222	3	7	1	253	252	-3	-3	2	419	439	-4	0	2	368	381	-6	3	2	304	324
5	3	1	242	215	4	7	1	262	258	-2	-3	2	552	575	-3	0	2	458	465	-5	3	2	370	359
6	3	1	211	227	-1	8	1	179	201	-1	-3	2	715	742	-2	0	2	495	528	-4	3	2	428	419
7	3	1	175	211	0	8	1	226	228	0	-3	2	722	720	-1	0	2	258	283	-3	3	2	460	441
-6	4	1	208	224	1	8	1	227	225	1	-3	2	587	577	0	0	2	279	355	-2	3	2	655	634
-5	4	1	280	283	2	8	1	261	265	2	-3	2	684	638	1	0	2	717	822	-1	3	2	282	294
-4	4	1	341	353	3	8	1	220	243	3	-3	2	550	513	2	0	2	321	-267	0	3	2	592	592
-3	4	1	448	424	4	8	1	204	213	4	-3	2	459	420	3	0	2	795	531	1	3	2	384	372
-2	4	1	490	486	-5	-6	2	196	226	5	-3	2	334	315	4	0	2	414	278	2	3	2	415	382
-1	4	1	541	523	-4	-6	2	204	241	6	-3	2	269	264	5	0	2	448	317	3	3	2	360	303
0	4	1	613	605	-3	-6	2	327	316	7	-3	2	194	212	6	0	2	269	244	4	3	2	267	244
1	4	1	436	432	-2	-6	2	304	272	8	-3	2	192	176	7	0	2	314	276	5	3	2	380	316
2	4	1	740	681	-1	-6	2	441	442	-6	-2	2	156	179	8	0	2	226	214	6	3	2	257	224
3	4	1	270	272	0	-6	2	290	283	-5	-2	2	201	216	9	0	2	171	180	7	3	2	213	221
4	4	1	440	401	1	-6	2	352	346	-4	-2	2	248	287	-7	1	2	184	205	8	3	2	192	205
5	4	1	359	325	2	-6	2	266	282	-3	-2	2	297	341	-6	1	2	243	241	-6	4	2	239	252
6	4	1	212	210	3	-6	2	268	296	-2	-2	2	445	492	-5	1	2	350	353	-5	4	2	335	339
7	4	1	202	191	5	-6	2	200	200	-1	-2	2	549	606	-4	1	2	370	374	-4	4	2	438	417
-6	5	1	189	188	-5	-5	2	205	211	0	-2	2	664	691	-3	1	2	474	460	-3	4	2	521	516
-5	5	1	160	202	-4	-5	2	190	216	1	-2	2	850	834	-2	1	2	572	597	-2	4	2	622	628
-4	5	1	258	274	-3	-5	2	305	320	2	-2	2	825	786	-1	1	2	589	602	-1	4	2	712	695
-3	5	1	230	240	-2	-5	2	308	304	3	-2	2	897	794	0	1	2	713	822	0	4	2	734	705
-2	5	1	323	321	-1	-5	2	363	362	4	-2	2	584	505	1	1	2	275	306	1	4	2	727	706
-1	5	1	355	357	0	-5	2	370	377	5	-2	2	742	613	2	1	2	1217	1050	2	4	2	582	531
0	5	1	324	321	1	-5	2	501	475	6	-2	2	392	364	3	1	2	476	379	3	4	2	618	549
1	5	1	357	348	2	-5	2	331	323	7	-2	2	328	312	4	1	2	571	459	4	4	2	460	413
2	5	1	443	423	3	-5	2	404	395	8	-2	2	230	237	5	1	2	552	422	5	4	2	336	295
3	5	1	290	296	4	-5	2	347	345	9	-2	2	204	187	6	1	2	361	305	6	4	2	242	222
4	5	1	378	372	5	-5	2	258	271	-7	-1	2	158	153	7	1	2	281	257	7	4	2	279	269
5	5	1	227	225	6	-5	2	234	220	-6	-1	2	206	241	8	1	2	212	219	-5	5	2	214	203
6	5	1	332	307	-6	-4	2	201	225	-5	-1	2	224	225	-7	2	2	215	205	-4	5	2	215	231
-6	6	1	181	205	-5	-4	2	323	342	-4	-1	2	213	221	-6	2	2	247	261	-3	5	2	328	322
-5	6	1	188	226	-4	-4	2	189	214	-3	-1	2	242	264	-5	2	2	188	196	-2	5	2	379	391
-4	6	1	266	274	-3	-4	2	421	440	-2	-1	2	147	155	-4	2	2	447	436	-1	5	2	435	438
-3	6	1	285	303	-2	-4	2	357	362	-1	-1	2	294	344	-3	2	2	260	260	0	5	2	565	554
-2	6	1	381	382	-1	-4	2	429	430	0	-1	2	155	179	-2	2	2	368	353	1	5	2	607	579
-1	6	1	174	178	0	-4	2	317	329	1	-1	2	397	392	-1	2	2	479	473	2	5	2	612	570
0	6	1	516	498	1	-4	2	513	492	2	-1	2	435	429	0	2	2	390	417	3	5	2	553	508

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(4-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
4	5	2	538	494	0	-5	3	403	388	-5	-1	3	171	177	-4	2	3	274	280	0	5	3	465	466
5	5	2	419	373	1	-5	3	439	421	-4	-1	3	237	255	-3	2	3	483	483	1	5	3	534	503
6	5	2	364	335	2	-5	3	426	409	-3	-1	3	222	255	-2	2	3	588	606	2	5	3	579	551
7	5	2	220	213	3	-5	3	495	472	-2	-1	3	244	261	-1	2	3	688	719	3	5	3	542	498
8	5	2	199	224	4	-5	3	244	261	-1	-1	3	262	290	0	2	3	638	691	4	5	3	523	457
-4	6	2	207	240	5	-5	3	342	340	0	-1	3	254	290	1	2	3	968	1021	5	5	3	426	391
-3	6	2	177	161	6	-5	3	189	222	1	-1	3	381	405	2	2	3	844	794	6	5	3	320	291
-2	6	2	257	258	-3	-4	3	267	296	2	-1	3	395	396	3	2	3	849	745	7	5	3	326	294
-1	6	2	272	276	-1	-4	3	353	354	3	-1	3	489	446	4	2	3	830	623	8	5	3	167	168
0	6	2	310	303	0	-4	3	225	215	4	-1	3	482	415	5	2	3	726	523	-2	6	3	167	180
1	6	2	214	213	1	-4	3	336	324	5	-1	3	533	439	6	2	3	562	396	0	6	3	162	162
2	6	2	454	441	2	-4	3	309	318	6	-1	3	393	342	7	2	3	325	305	1	6	3	369	366
3	6	2	265	275	3	-4	3	398	365	7	-1	3	337	308	8	2	3	209	251	2	6	3	178	168
4	6	2	300	293	4	-4	3	348	344	8	-1	3	242	234	-6	3	3	237	242	3	6	3	356	334
5	6	2	329	304	5	-4	3	320	316	9	-1	3	257	221	-5	3	3	211	193	4	6	3	329	328
6	6	2	254	252	6	-4	3	281	279	-7	0	3	229	226	-4	3	3	430	419	5	6	3	322	293
7	6	2	190	198	7	-4	3	229	244	-6	0	3	297	294	-3	3	3	302	300	6	6	3	260	249
-4	7	2	188	183	-6	-3	3	194	196	-5	0	3	352	356	-2	3	3	436	429	7	6	3	249	241
-3	7	2	201	225	-5	-3	3	239	281	-4	0	3	386	393	-1	3	3	449	463	-2	7	3	181	179
-2	7	2	207	251	-4	-3	3	182	232	-3	0	3	462	479	0	3	3	606	609	0	7	3	181	201
-1	7	2	217	215	-3	-3	3	277	284	-2	0	3	240	252	1	3	3	440	434	2	7	3	260	246
0	7	2	340	336	-2	-3	3	344	391	-1	0	3	588	640	2	3	3	644	592	4	7	3	157	157
1	7	2	237	229	-1	-3	3	310	320	0	0	3	139	164	3	3	3	622	553	0	8	3	191	196
2	7	2	279	277	0	-3	3	201	209	1	0	3	260	321	4	3	3	638	507	0	-6	4	202	214
3	7	2	219	210	1	-3	3	517	488	2	0	3	124	126	5	3	3	550	425	2	-6	4	177	191
4	7	2	269	273	2	-3	3	209	205	3	0	3	577	513	6	3	3	463	366	-3	-5	4	203	192
6	7	2	196	200	3	-3	3	332	303	5	0	3	460	345	7	3	3	382	325	-2	-5	4	242	241
8	7	2	201	135	4	-3	3	282	266	6	0	3	299	248	8	3	3	269	242	-1	-5	4	255	251
-2	8	2	216	185	5	-3	3	253	247	7	0	3	298	233	9	3	3	194	202	0	-5	4	272	260
0	8	2	218	215	6	-3	3	250	246	8	0	3	226	219	-6	4	3	203	209	1	-5	4	362	340
1	8	2	214	229	7	-3	3	163	192	9	0	3	204	187	-5	4	3	259	270	2	-5	4	312	285
2	8	2	206	229	8	-3	3	164	183	-7	1	3	221	241	-4	4	3	325	328	3	-5	4	258	250
3	8	2	207	203	-5	-2	3	247	259	-6	1	3	276	288	-3	4	3	415	415	4	-5	4	271	264
4	8	2	211	218	-4	-2	3	249	269	-5	1	3	381	397	-2	4	3	492	486	5	-5	4	196	226
-2	-7	3	188	172	-3	-2	3	334	362	-4	1	3	490	489	-1	4	3	498	493	-2	-4	4	184	175
0	-7	3	167	171	-2	-2	3	343	385	-3	1	3	619	630	0	4	3	601	590	-1	-4	4	184	191
-4	-6	3	219	216	-1	-2	3	425	476	-2	1	3	731	739	1	4	3	581	565	0	-4	4	178	166
-3	-6	3	259	280	0	-2	3	502	535	-1	1	3	730	783	2	4	3	555	509	1	-4	4	258	257
-2	-6	3	303	293	1	-2	3	503	500	0	1	3	696	797	3	4	3	624	559	2	-4	4	302	292
-1	-6	3	325	318	2	-2	3	562	524	1	1	3	794	947	4	4	3	311	276	3	-4	4	270	279
0	-6	3	297	286	3	-2	3	517	476	2	1	3	432	450	5	4	3	557	453	4	-4	4	302	298
1	-6	3	349	345	4	-2	3	472	429	3	1	3	550	557	6	4	3	293	264	5	-4	4	259	281
2	-6	3	257	250	5	-2	3	383	354	4	1	3	487	425	7	4	3	271	243	6	-4	4	264	252
3	-6	3	224	194	6	-2	3	272	260	5	1	3	445	347	8	4	3	215	198	7	-4	4	178	210
4	-6	3	214	232	7	-2	3	288	263	6	1	3	231	196	-4	5	3	204	204	-6	-3	4	169	185
-3	-5	3	235	239	8	-2	3	185	194	7	1	3	330	275	-3	5	3	247	275	-4	-3	4	183	194
-2	-5	3	264	276	-7	-1	3	162	176	-6	2	3	178	206	-2	5	3	314	314	-3	-3	4	312	351
-1	-5	3	367	398	-6	-1	3	216	221	-5	2	3	333	347	-1	5	3	439	434	-1	-3	4	267	286

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(4-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
0	-3	4	174	164	7	0	4	382	303	8	3	4	363	290	2	9	4	207	198	5	-1	5	435	399
1	-3	4	198	178	8	0	4	289	253	9	3	4	232	219	-2	-5	5	187	202	6	-1	5	394	343
3	-3	4	272	259	9	0	4	216	199	-5	4	4	208	202	0	-5	5	226	233	7	-1	5	273	244
5	-3	4	199	203	-7	1	4	188	195	-4	4	4	221	229	2	-5	5	163	173	8	-1	5	193	194
6	-3	4	198	196	-6	1	4	233	235	-3	4	4	224	218	3	-5	5	181	166	-4	0	5	207	208
7	-3	4	174	188	-5	1	4	337	337	-2	4	4	240	247	6	-5	5	174	154	-3	0	5	244	224
-7	-2	4	173	188	-4	1	4	423	415	-1	4	4	244	249	-3	-4	5	181	202	-2	0	5	287	287
-6	-2	4	229	219	-3	1	4	499	504	0	4	4	290	281	-2	-4	5	242	256	-1	0	5	336	348
-5	-2	4	303	296	-2	1	4	557	567	1	4	4	215	228	0	-4	5	377	368	0	0	5	488	541
-4	-2	4	290	333	-1	1	4	712	726	2	4	4	288	282	1	-4	5	264	246	1	0	5	377	450
-3	-2	4	377	419	0	1	4	592	668	3	4	4	319	302	2	-4	5	339	320	2	0	5	530	615
-2	-2	4	402	462	1	1	4	580	726	4	4	4	317	304	3	-4	5	281	265	3	0	5	557	585
-1	-2	4	464	507	2	1	4	404	483	5	4	4	365	323	4	-4	5	270	274	4	0	5	635	624
0	-2	4	417	432	3	1	4	779	842	6	4	4	253	230	5	-4	5	227	235	5	0	5	409	401
1	-2	4	496	478	4	1	4	170	185	7	4	4	348	290	-4	-3	5	187	200	6	0	5	583	499
2	-2	4	404	374	5	1	4	511	486	8	4	4	234	224	-3	-3	5	173	202	7	0	5	392	322
3	-2	4	320	304	6	1	4	347	286	-4	5	4	230	220	-2	-3	5	202	224	8	0	5	325	275
4	-2	4	297	268	7	1	4	363	266	-3	5	4	249	248	-1	-3	5	327	345	9	0	5	224	212
5	-2	4	198	200	8	1	4	199	202	-2	5	4	285	287	1	-3	5	311	295	-6	1	5	199	182
6	-2	4	232	234	9	1	4	202	194	-1	5	4	312	308	2	-3	5	312	295	-5	1	5	192	188
-5	-1	4	295	294	-5	2	4	246	233	0	5	4	311	317	3	-3	5	211	199	-4	1	5	269	238
-4	-1	4	278	294	-4	2	4	259	246	1	5	4	356	368	4	-3	5	278	272	-3	1	5	274	264
-3	-1	4	369	377	-3	2	4	532	535	2	5	4	307	292	5	-3	5	246	243	-2	1	5	320	291
-2	-1	4	445	465	-2	2	4	360	360	3	5	4	367	344	6	-3	5	198	221	-1	1	5	364	354
-1	-1	4	472	540	-1	2	4	725	735	4	5	4	254	242	8	-3	5	180	167	0	1	5	219	242
0	-1	4	532	626	0	2	4	675	749	5	5	4	334	295	-6	-2	5	175	176	1	1	5	375	481
1	-1	4	573	618	1	2	4	767	858	6	5	4	209	204	-5	-2	5	240	257	2	1	5	295	331
2	-1	4	632	627	2	2	4	744	789	7	5	4	231	219	-4	-2	5	297	316	3	1	5	338	369
3	-1	4	602	568	3	2	4	797	798	-4	6	4	181	128	-3	-2	5	359	386	4	1	5	336	372
4	-1	4	547	486	4	2	4	759	653	-3	6	4	186	185	-2	-2	5	372	399	5	1	5	415	450
5	-1	4	472	422	5	2	4	632	532	-1	6	4	240	247	-1	-2	5	402	444	6	1	5	256	263
6	-1	4	347	301	6	2	4	489	396	0	6	4	197	207	0	-2	5	438	463	7	1	5	354	310
7	-1	4	326	293	7	2	4	442	345	1	6	4	250	249	1	-2	5	446	424	8	1	5	308	268
8	-1	4	177	205	8	2	4	202	232	2	6	4	202	213	2	-2	5	357	327	9	1	5	194	188
-7	0	4	169	174	9	2	4	204	197	3	6	4	399	378	3	-2	5	409	364	-5	2	5	211	225
-6	0	4	231	252	-5	3	4	176	168	4	6	4	157	168	4	-2	5	267	252	-4	2	5	233	235
-5	0	4	261	251	-4	3	4	201	175	5	6	4	302	284	5	-2	5	208	228	-3	2	5	267	259
-4	0	4	355	329	-3	3	4	159	152	6	6	4	224	223	6	-2	5	203	204	-2	2	5	359	354
-3	0	4	386	389	-2	3	4	315	311	7	6	4	209	195	-5	-1	5	241	229	-1	2	5	465	460
-2	0	4	410	421	-1	3	4	309	326	0	7	4	143	148	-4	-1	5	230	230	0	2	5	354	371
-1	0	4	507	526	0	3	4	236	254	1	7	4	184	181	-3	-1	5	432	443	1	2	5	434	504
0	0	4	271	328	1	3	4	616	638	4	7	4	156	170	-2	-1	5	404	443	2	2	5	433	474
1	0	4	572	694	2	3	4	462	454	7	7	4	166	171	-1	-1	5	540	572	3	2	5	433	473
2	0	4	403	454	3	3	4	622	580	-2	8	4	186	201	0	-1	5	573	648	4	2	5	357	362
3	0	4	368	388	4	3	4	640	530	0	8	4	176	180	1	-1	5	621	673	5	2	5	380	391
4	0	4	578	537	5	3	4	622	515	1	8	4	193	205	2	-1	5	668	693	6	2	5	316	298
5	0	4	448	398	6	3	4	552	437	2	8	4	173	191	3	-1	5	592	577	7	2	5	278	272
6	0	4	417	332	7	3	4	421	342	0	9	4	176	204	4	-1	5	558	524	8	2	5	190	204

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [H(4-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
9	2	5	220	196	2	7	5	167	168	0	-1	6	374	402	0	3	6	257	257	5	7	6	322	310
-3	3	5	283	285	3	7	5	366	357	1	-1	6	398	421	1	3	6	374	421	7	7	6	182	192
-1	3	5	308	307	5	7	5	234	253	2	-1	6	424	423	2	3	6	399	435	8	7	6	183	159
0	3	5	276	274	6	7	5	200	179	3	-1	6	412	394	3	3	6	298	322	3	8	6	190	169
1	3	5	385	419	7	7	5	174	179	4	-1	6	381	365	4	3	6	305	319	-2	-4	7	197	206
2	3	5	234	256	0	8	5	195	204	5	-1	6	308	301	5	3	6	277	302	-1	-4	7	203	191
3	3	5	542	553	1	8	5	178	185	6	-1	6	293	269	6	3	6	245	246	0	-4	7	249	228
4	3	5	367	364	1	9	5	216	204	7	-1	6	193	199	7	3	6	205	206	1	-4	7	284	261
5	3	5	433	399	-1	-5	6	181	175	8	-1	6	198	204	8	3	6	176	173	2	-4	7	223	221
6	3	5	371	334	0	-5	6	187	180	-3	0	6	220	190	-3	4	6	240	212	3	-4	7	209	211
7	3	5	334	301	1	-5	6	194	148	-2	0	6	223	194	-2	4	6	203	215	0	-3	7	286	276
8	3	5	298	242	2	-5	6	207	183	-1	0	6	264	232	-1	4	6	261	258	1	-3	7	165	151
-4	4	5	211	181	-4	-4	6	218	202	0	0	6	310	324	0	4	6	283	287	2	-3	7	430	392
-2	4	5	225	218	-2	-4	6	251	283	1	0	6	260	312	1	4	6	314	326	3	-3	7	264	255
-1	4	5	163	152	-1	-4	6	277	292	2	0	6	486	533	2	4	6	226	248	4	-3	7	318	290
0	4	5	151	145	0	-4	6	342	350	3	0	6	331	354	3	4	6	361	371	5	-3	7	255	263
1	4	5	199	195	1	-4	6	309	282	4	0	6	456	478	4	4	6	284	283	6	-3	7	245	234
2	4	5	167	170	2	-4	6	381	356	5	0	6	401	408	5	4	6	292	291	0	-2	7	157	137
3	4	5	213	200	3	-4	6	277	273	6	0	6	376	354	6	4	6	256	261	1	-2	7	166	159
4	4	5	219	221	4	-4	6	274	253	7	0	6	294	277	7	4	6	239	207	3	-2	7	198	185
5	4	5	223	214	5	-4	6	174	193	8	0	6	256	247	8	4	6	221	224	4	-2	7	260	260
6	4	5	321	286	6	-4	6	166	176	9	0	6	196	185	-4	5	6	199	172	5	-2	7	191	193
7	4	5	216	202	-2	-3	6	236	240	-6	1	6	174	134	-3	5	6	273	269	6	-2	7	252	235
8	4	5	229	207	-1	-3	6	183	155	-4	1	6	186	171	-2	5	6	278	268	8	-2	7	196	174
9	4	5	189	179	0	-3	6	376	387	-2	1	6	171	144	-1	5	6	302	289	-3	-1	7	183	158
-5	5	5	218	212	1	-3	6	314	298	-1	1	6	144	131	0	5	6	303	295	-2	-1	7	286	243
-4	5	5	249	232	2	-3	6	372	346	0	1	6	183	168	1	5	6	327	310	-1	-1	7	172	146
-3	5	5	284	265	3	-3	6	334	326	1	1	6	133	146	2	5	6	289	281	0	-1	7	232	204
-2	5	5	321	296	4	-3	6	405	389	3	1	6	208	246	3	5	6	273	250	1	-1	7	185	172
-1	5	5	308	311	5	-3	6	255	253	4	1	6	297	332	4	5	6	265	250	2	-1	7	183	186
0	5	5	304	301	6	-3	6	293	282	5	1	6	167	160	5	5	6	199	206	3	-1	7	188	162
1	5	5	279	266	7	-3	6	210	211	6	1	6	369	380	6	5	6	240	208	4	-1	7	156	161
2	5	5	247	238	8	-3	6	170	173	7	1	6	209	234	7	5	6	184	175	-4	0	7	201	166
3	5	5	265	237	-3	-2	6	209	199	8	1	6	221	240	-2	6	6	259	268	-3	0	7	212	202
5	5	5	222	217	-2	-2	6	239	239	9	1	6	220	191	-1	6	6	289	286	-2	0	7	239	183
-3	6	5	196	218	-1	-2	6	290	297	-5	2	6	185	197	0	6	6	376	370	-1	0	7	301	279
-2	6	5	245	255	0	-2	6	236	231	-4	2	6	253	223	1	6	6	343	342	0	0	7	283	292
-1	6	5	335	335	1	-2	6	309	292	-3	2	6	278	269	2	6	6	363	342	1	0	7	264	286
0	6	5	281	271	2	-2	6	327	317	-2	2	6	354	333	3	6	6	359	344	2	0	7	283	297
1	6	5	384	388	3	-2	6	280	271	-1	2	6	221	190	4	6	6	320	316	3	0	7	261	284
2	6	5	354	341	4	-2	6	238	266	0	2	6	344	353	5	6	6	231	207	4	0	7	282	301
3	6	5	281	265	5	-2	6	300	277	1	2	6	198	232	6	6	6	238	240	5	0	7	204	229
4	6	5	308	300	6	-2	6	241	232	2	2	6	169	226	7	6	6	176	172	6	0	7	194	211
5	6	5	286	259	7	-2	6	233	219	3	2	6	175	202	0	7	6	156	167	7	0	7	196	212
6	6	5	178	171	-4	-1	6	232	222	5	2	6	186	228	1	7	6	284	290	-2	1	7	217	193
-1	7	5	173	205	-3	-1	6	273	238	-3	3	6	265	260	2	7	6	265	257	-1	1	7	222	188
0	7	5	215	211	-2	-1	6	314	289	-2	3	6	252	248	3	7	6	295	285	0	1	7	229	222
1	7	5	255	254	-1	-1	6	395	383	-1	3	6	493	480	4	7	6	254	238	1	1	7	160	180

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR [N(4-picNO)2][AuCl4]

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	1	7	296	341	6	4	7	285	294	0	0	8	320	301	1	4	8	326	319	4	0	9	187	200
3	1	7	179	178	7	4	7	274	257	1	0	8	305	311	2	4	8	246	287	6	0	9	151	140
4	1	7	258	304	8	4	7	187	190	2	0	8	276	290	3	4	8	282	304	-2	1	9	209	172
5	1	7	186	244	-1	5	7	216	197	3	0	8	278	272	4	4	8	323	363	-1	1	9	262	212
6	1	7	269	299	0	5	7	231	225	4	0	8	196	188	5	4	8	253	258	0	1	9	246	236
8	1	7	201	244	1	5	7	247	229	5	0	8	191	211	6	4	8	245	270	1	1	9	262	294
-5	2	7	196	162	2	5	7	241	257	-2	1	8	234	195	7	4	8	196	214	2	1	9	309	312
-4	2	7	281	249	3	5	7	283	283	-1	1	8	299	280	8	4	8	164	178	3	1	9	319	334
-3	2	7	254	215	4	5	7	271	279	0	1	8	334	319	1	5	8	157	141	4	1	9	264	266
-2	2	7	316	284	5	5	7	246	251	1	1	8	299	335	2	5	8	175	177	5	1	9	236	287
-1	2	7	322	281	6	5	7	279	271	2	1	8	337	370	3	5	8	176	188	6	1	9	220	228
0	2	7	312	312	7	5	7	183	186	3	1	8	282	321	4	5	8	194	212	7	1	9	201	200
1	2	7	192	206	8	5	7	220	216	4	1	8	370	396	5	5	8	231	231	-1	2	9	201	129
2	2	7	234	278	-1	6	7	188	188	5	1	8	237	265	6	5	8	211	215	0	2	9	164	142
3	2	7	186	210	0	6	7	229	219	6	1	8	203	248	7	5	8	210	198	1	2	9	158	174
4	2	7	189	216	1	6	7	211	199	7	1	8	213	246	8	5	8	180	180	2	2	9	204	193
6	2	7	186	205	2	6	7	287	275	-2	2	8	243	221	0	7	8	161	143	3	2	9	235	250
7	2	7	162	176	3	6	7	205	201	-1	2	8	239	198	0	-3	9	176	150	4	2	9	201	264
-5	3	7	190	172	4	6	7	235	221	0	2	8	237	231	0	-2	9	187	166	5	2	9	201	241
-3	3	7	314	294	5	6	7	204	221	1	2	8	276	292	1	-2	9	226	200	6	2	9	221	246
-2	3	7	404	367	6	6	7	161	188	2	2	8	254	281	2	-2	9	208	210	7	2	9	206	217
-1	3	7	344	302	1	7	7	192	194	3	2	8	254	268	4	-2	9	230	219	8	2	9	166	192
0	3	7	450	484	3	7	7	206	207	4	2	8	274	298	5	-2	9	183	168	4	3	9	181	181
1	3	7	416	438	4	7	7	268	250	5	2	8	221	258	-2	-1	9	200	159	0	4	9	171	179
2	3	7	352	412	6	7	7	208	216	6	2	8	232	278	-1	-1	9	193	158	3	5	9	175	152
3	3	7	327	337	0	-3	8	173	155	8	2	8	179	223	0	-1	9	161	140	0	7	9	150	141
4	3	7	374	405	1	-3	8	221	205	-2	3	8	257	222	1	-1	9	198	170	0	-2	10	185	168
5	3	7	216	221	2	-3	8	181	171	-1	3	8	271	241	3	-1	9	189	176	3	-2	10	234	222
6	3	7	216	241	4	-3	8	191	195	0	3	8	357	369	4	-1	9	165	167	3	-1	10	191	174
7	3	7	193	187	0	-2	8	160	137	1	3	8	169	171	6	-1	9	199	168	4	-1	10	219	192
-2	4	7	226	211	2	-2	8	231	199	2	3	8	365	408	-3	0	9	212	164	5	-1	10	197	181
-1	4	7	341	339	5	-2	8	172	173	3	3	8	216	267	-2	0	9	244	185	6	-1	10	159	163
0	4	7	294	274	6	-2	8	203	198	4	3	8	246	278	-1	0	9	189	189	0	1	10	154	160
1	4	7	376	408	-2	-1	8	217	160	5	3	8	202	238	0	0	9	316	288	0	4	10	178	140
2	4	7	395	413	0	-1	8	205	185	6	3	8	207	243	1	0	9	225	214	-1	5	10	221	153
3	4	7	408	422	-3	0	8	222	205	-2	4	8	177	150	2	0	9	274	237	0	5	10	155	137
4	4	7	347	365	-2	0	8	316	297	-1	4	8	181	189	3	0	9	212	226	0	4	11	178	143
5	4	7	386	371	-1	0	8	294	266	0	4	8	240	233										